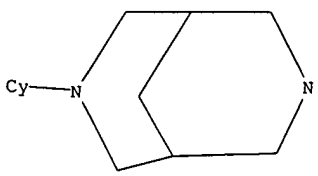
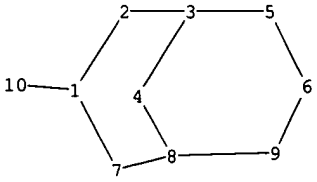
C:\STNEXP4\QUERIES\09864905.str




chain nodes :
    10
ring nodes :
    1  2  3  4  5  6  7  8  9
chain bonds :
    1-10
ring bonds :
    1-2  1-7  2-3  3-4  3-5  4-8  5-6  6-9  7-8  8-9
exact/norm bonds :
    1-2  1-7  1-10  2-3  3-4  3-5  4-8  5-6  6-9  7-8  8-9
isolated ring systems :
    containing 1 :

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom
    10:Atom

Welcome to STN International! Enter x:x

LOGINID:ssspta1611hxl

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

```
 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2  Apr 08  "Ask CAS" for self-help around the clock
 NEWS  3  Apr 09  BEILSTEIN: Reload and Implementation of a New Subject Area
 NEWS  4  Apr 09  ZDB will be removed from STN
 NEWS  5  Apr 19  US Patent Applications available in IFICDB, IFIPAT, and
IFIUDB
 NEWS  6  Apr 22  Records from IP.com available in CAPLUS, HCAPLUS, and
ZCAPLUS
 NEWS  7  Apr 22  BIOSIS Gene Names now available in TOXCENTER
 NEWS  8  Apr 22  Federal Research in Progress (FEDRIP) now available
 NEWS  9  Jun 03  New e-mail delivery for search results now available
 NEWS 10  Jun 10  MEDLINE Reload
 NEWS 11  Jun 10  PCTFULL has been reloaded
 NEWS 12  Jul 02  FOREGE no longer contains STANDARDS file segment
 NEWS 13  Jul 22  USAN to be reloaded July 28, 2002;
                  saved answer sets no longer valid
 NEWS 14  Jul 29  Enhanced polymer searching in REGISTRY
 NEWS 15  Jul 30  NETFIRST to be removed from STN
 NEWS 16  Aug 08  CANCERLIT reload
 NEWS 17  Aug 08  PHARMAMarketLetter(PHARMAML) - new on STN
 NEWS 18  Aug 08  NTIS has been reloaded and enhanced
 NEWS 19  Aug 19  Aquatic Toxicity Information Retrieval (AQUIRE)
                  now available on STN
 NEWS 20  Aug 19  IFIPAT, IFICDB, and IFIUDB have been reloaded
 NEWS 21  Aug 19  The MEDLINE file segment of TOXCENTER has been reloaded
 NEWS 22  Aug 26  Sequence searching in REGISTRY enhanced
 NEWS 23  Sep 03  JAPIO has been reloaded and enhanced
 NEWS 24  Sep 16  Experimental properties added to the REGISTRY file
 NEWS 25  Sep 16  Indexing added to some pre-1967 records in CA/CAPLUS
 NEWS 26  Sep 16  CA Section Thesaurus available in CAPLUS and CA

 NEWS EXPRESS  February 1 CURRENT WINDOWS VERSION IS V6.0d,
               CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
               AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:35:52 ON 22 SEP 2002

=> fil reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 11:36:00 ON 22 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593-49-2
DICTIONARY FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593-49-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

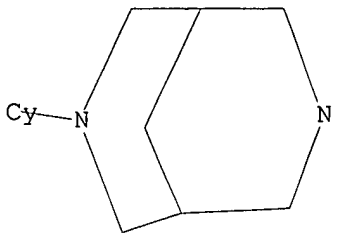
=>
Uploading C:\STNEXP4\QUERIES\09864905.str

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

```
=> d l1
L1 HAS NO ANSWERS
L1                STR
```




Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 11:36:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   9550 TO ITERATE

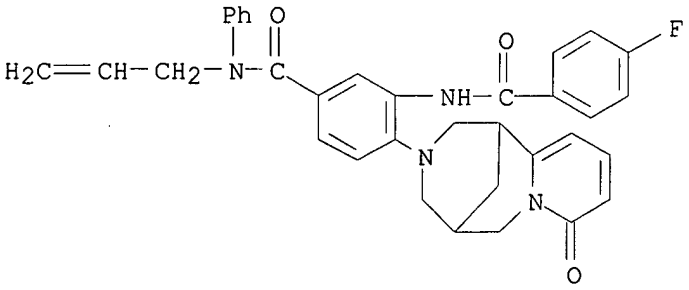
 10.5% PROCESSED    1000 ITERATIONS                                 6 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       185150 TO   196850
PROJECTED ANSWERS:             692 TO     1600

L3            6 SEA SSS SAM L1

=> d scan

L3   6 ANSWERS   REGISTRY  COPYRIGHT 2002 ACS
IN   Benzamide, 3-[(4-fluorobenzoyl)amino]-N-phenyl-N-2-propenyl-4-(1,5,6,8-
     tetrahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-yl)-
     (9CI)
MF   C34 H31 F N4 O3
```

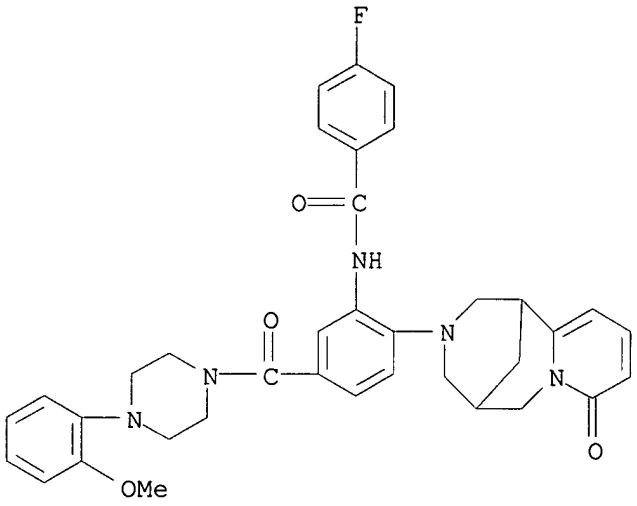



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

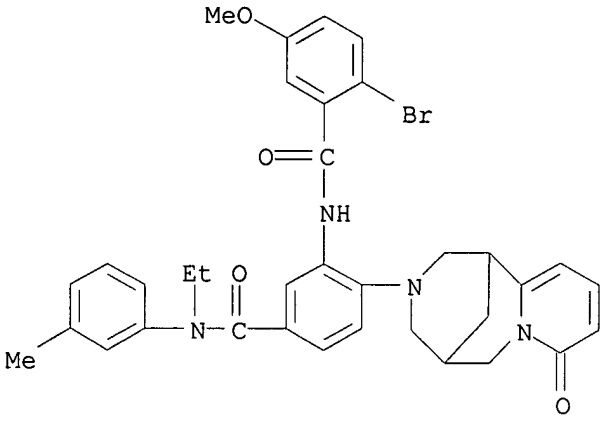
L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide, 4-fluoro-N-[5-[[4-(2-methoxyphenyl)-1-piperazinyl]carbonyl]-2-

(1,5,6,8-tetrahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-yl)phenyl]- (9CI)
MF C36 H36 F N5 O4




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

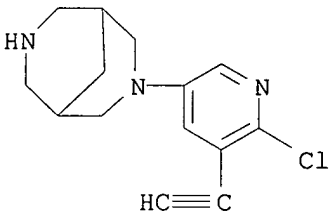
L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide,
3-[(2-bromo-5-methoxybenzoyl)amino]-N-ethyl-N-(3-methylphenyl)-4-(1,5,6,8-tetrahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-yl)- (9CI)
MF C35 H35 Br N4 O4




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

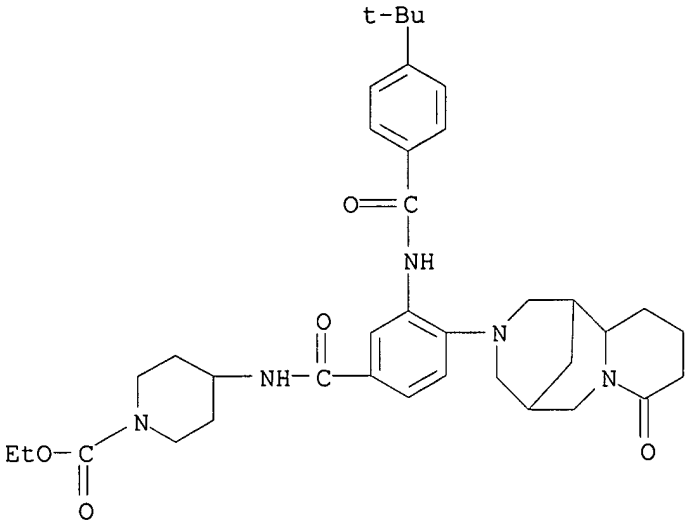
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-ethynyl-3-pyridinyl)- (9CI)
MF C14 H16 Cl N3




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1-Piperidinecarboxylic acid,
4-[[3-[[4-(1,1-dimethylethyl)benzoyl]amino]-4-
(octahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-
yl)benzoyl]amino]-, ethyl ester (9CI)
MF C37 H49 N5 O5




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

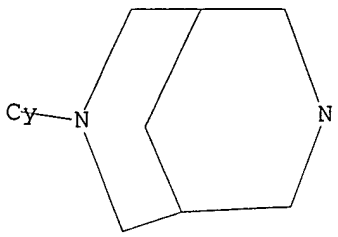
=>
Uploading C:\STNEXP4\QUERIES\09864905.str

L4 STRUCTURE UPLOADED

=> que L4

L5 QUE L4

=> d l4
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l4
SAMPLE SEARCH INITIATED 11:38:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    283 TO ITERATE

100.0% PROCESSED     283 ITERATIONS                          5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         4651 TO     6669
PROJECTED ANSWERS:               5 TO      234

L6            5 SEA SSS SAM L4

=> s l6 ful
FULL SEARCH INITIATED 11:39:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   5707 TO ITERATE

100.0% PROCESSED    5707 ITERATIONS                       100 ANSWERS
SEARCH TIME: 00.00.01

L7          100 SEA SSS FUL L4

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               141.80     142.01

FILE 'CAPLUS' ENTERED AT 11:39:10 ON 22 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 22 Sep 2002  VOL 137 ISS 13
FILE LAST UPDATED: 20 Sep 2002  (20020920/ED)
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This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

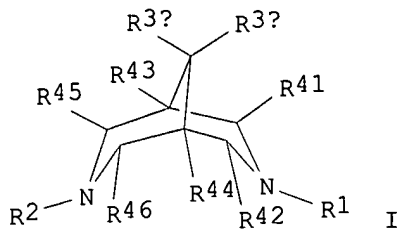
=> s l7
L8 28 L7

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 28 ANSWERS - CONTINUE? Y/(N):y

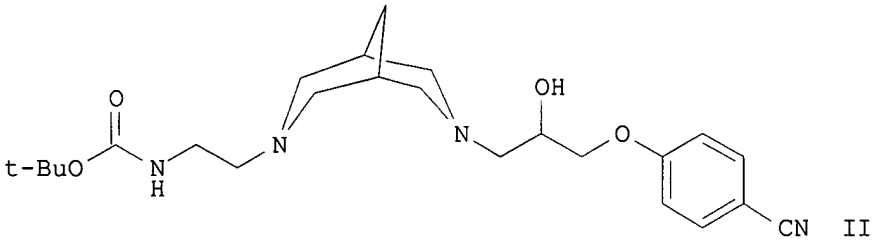
L8 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:51458 CAPLUS
DOCUMENT NUMBER: 136:118479
TITLE: Preparation of new bispidine compounds for the treatment of cardiac arrhythmias
INVENTOR(S): Andersson, Kjell; Bjoere, Annika; Bjoersne, Magnus; Ponten, Fritiof; Strandlund, Gert; Svensson, Peder; Tottie, Louise
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002004446 | A1 | 20020117 | WO 2001-SE1544 | 20010704 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2001071161 | A5 | 20020121 | AU 2001-71161 | 20010704 |

PRIORITY APPLN. INFO.: SE 2000-2603 A 20000707
SE 2000-2788 A 20000727
WO 2001-SE1544 W 20010704
OTHER SOURCE(S): MARPAT 136:118479
GI




I




II

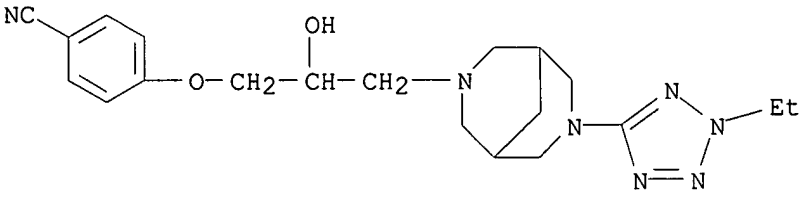
AB The title compds. [I; R1 = ACR4R5BR6 (wherein R4 = H, halo, alkyl, etc.; or R4, together with R5, = O; R5 = H, alkyl,; A = a bond, alkylene, etc.; B = a bond, alkylene, etc.; R6 = (un)substituted aryl, 5-12 membered heterocyclyl contg. one or more heteroatoms selected from O, N and/or S); R2 = CN, (un)substituted 5-12 membered heterocyclyl contg. one or more heteroatoms selected from O, N and/or S, etc.; R3a, R3b = H, alkyl, etc.; or R3a and R3b together = alkylene, O(alkylene)O, etc.; R41-R46 = H, alkyl] which are useful in the prophylaxis and in the treatment of arrhythmias, in particular atrial and ventricular arrhythmias, were prepd.

E.g., a 3-step synthesis of II was given. The exemplified compds. I showed pIC50 of at least 5.5 in glucocorticoid-treated mouse fibroblasts as a model to detect blockers of the delayed rectifier K current.

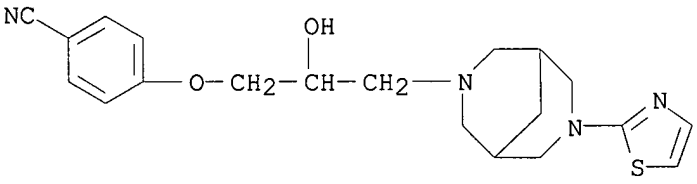
IT **389885-68-1P 389885-69-2P 389886-19-5P**
**389886-27-5P 389886-28-6P 389886-29-7P**
**389886-44-6P 389886-54-8P 389886-70-8P**
**389886-88-8P 389886-89-9P 389886-90-2P**
**389886-91-3P 389887-29-0P 389887-30-3P**
**389887-66-5P 389887-67-6P 389887-68-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of new bispidine compds. for the treatment of cardiac arrhythmias)

RN 389885-68-1 CAPLUS

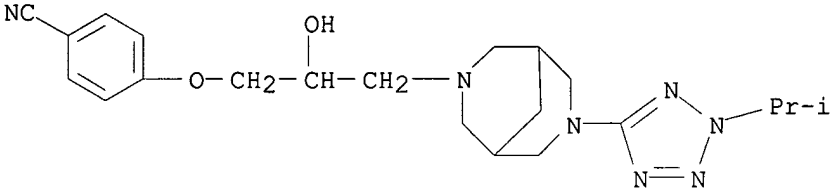
CN Benzonitrile, 4-[3-[7-(2-ethyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)



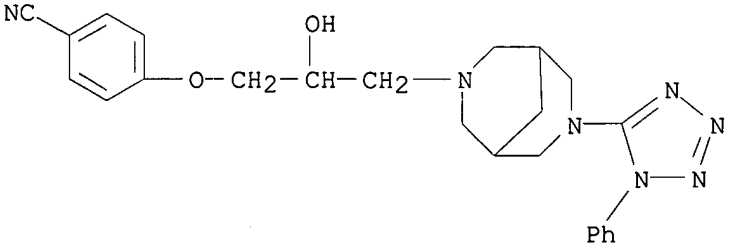
RN 389885-69-2 CAPLUS
CN Benzonitrile,
4-[2-hydroxy-3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



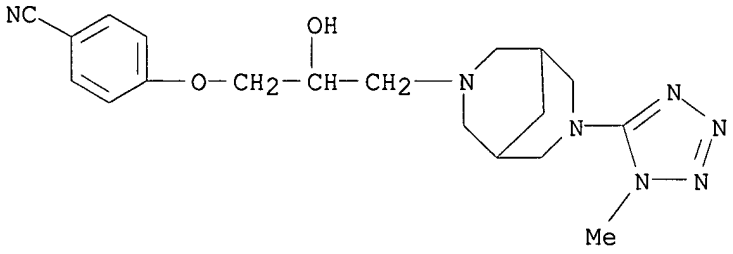
RN 389886-19-5 CAPLUS
CN Benzonitrile, 4-[2-hydroxy-3-[7-[2-(1-methylethyl)-2H-tetrazol-5-yl]-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



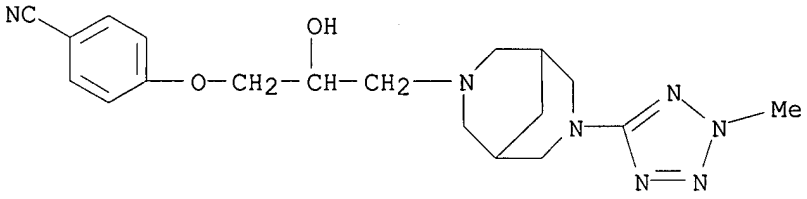
RN 389886-27-5 CAPLUS
CN Benzonitrile, 4-[2-hydroxy-3-[7-(1-phenyl-1H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



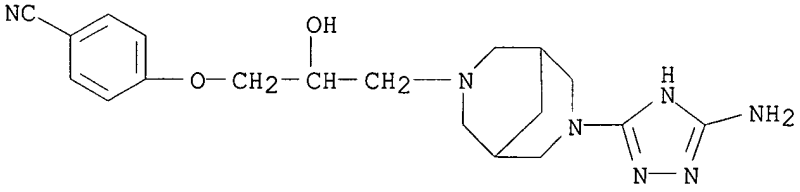
RN 389886-28-6 CAPLUS
CN Benzonitrile, 4-[2-hydroxy-3-[7-(1-methyl-1H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



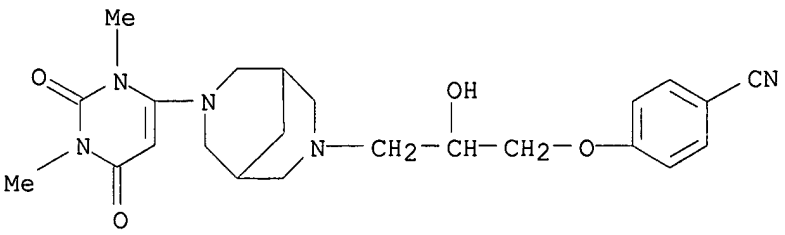
RN 389886-29-7 CAPLUS
CN Benzonitrile, 4-[2-hydroxy-3-[7-(2-methyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



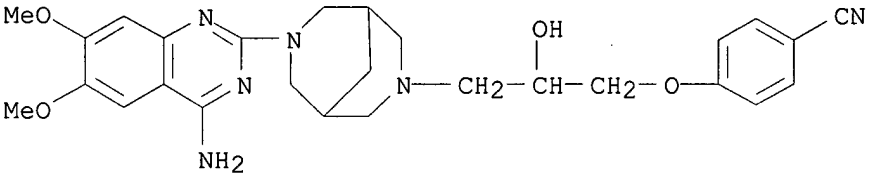
RN 389886-44-6 CAPLUS
CN Benzonitrile, 4-[3-[7-(5-amino-1H-1,2,4-triazol-3-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)



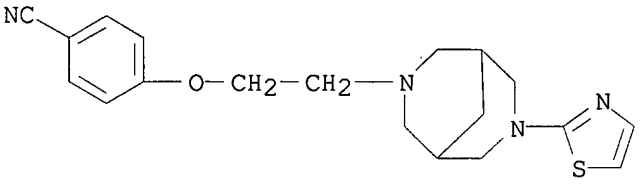
RN 389886-54-8 CAPLUS
CN Benzonitrile,
4-[2-hydroxy-3-[7-(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



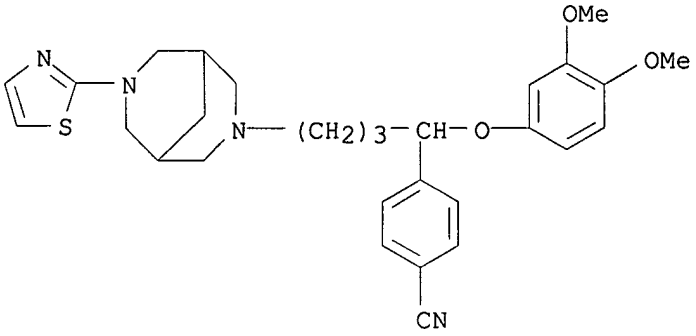
RN 389886-70-8 CAPLUS
CN Benzonitrile, 4-[3-[7-(4-amino-6,7-dimethoxy-2-quinazolinyl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)



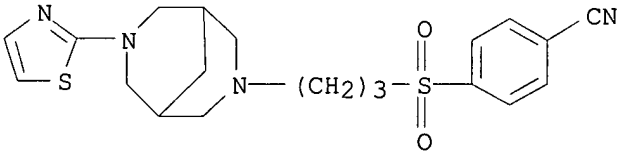
RN 389886-88-8 CAPLUS
CN Benzonitrile, 4-[2-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]ethoxy]- (9CI) (CA INDEX NAME)



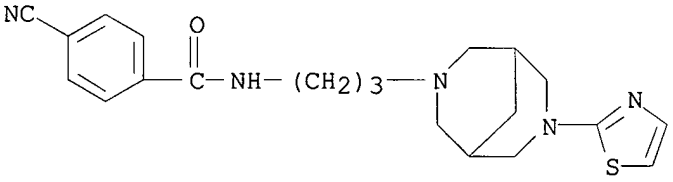
RN 389886-89-9 CAPLUS
CN Benzonitrile, 4-[1-(3,4-dimethoxyphenoxy)-4-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]butyl]- (9CI) (CA INDEX NAME)



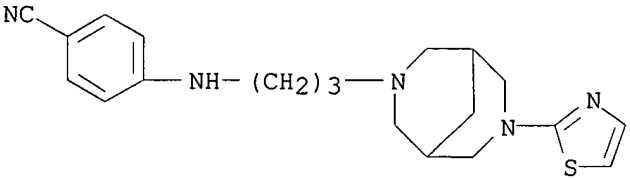
RN 389886-90-2 CAPLUS
CN Benzonitrile, 4-[[3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]sulfonyl]- (9CI) (CA INDEX NAME)



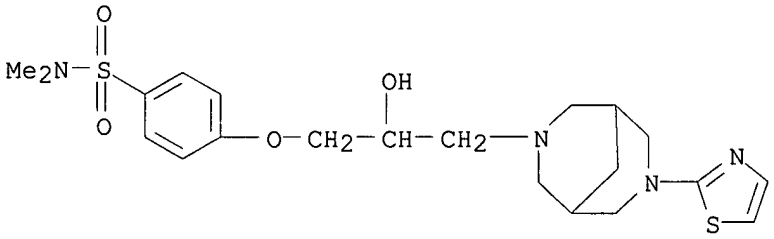
RN 389886-91-3 CAPLUS
CN Benzamide, 4-cyano-N-[3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]- (9CI) (CA INDEX NAME)



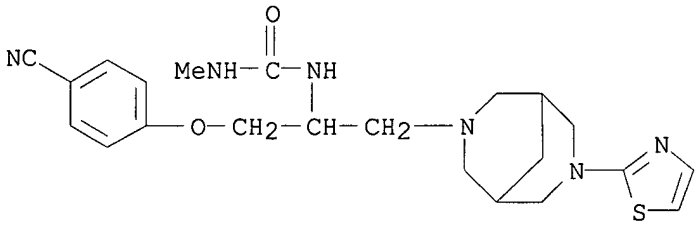
RN 389887-29-0 CAPLUS
CN Benzonitrile, 4-[[3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]amino]- (9CI) (CA INDEX NAME)



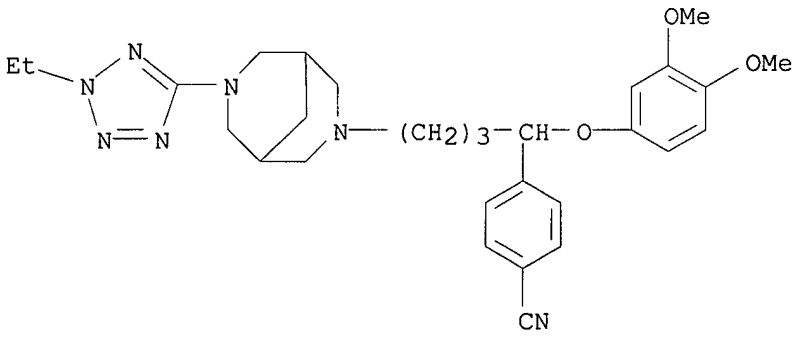
RN 389887-30-3 CAPLUS
CN Benzenesulfonamide, 4-[2-hydroxy-3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



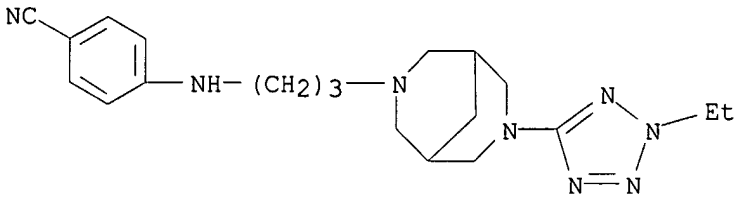
RN 389887-66-5 CAPLUS
CN Urea, N-[1-[(4-cyanophenoxy)methyl]-2-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]ethyl]-N'-methyl- (9CI) (CA INDEX NAME)



RN 389887-67-6 CAPLUS
CN Benzonitrile, 4-[1-(3,4-dimethoxyphenoxy)-4-[7-(2-ethyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]butyl]- (9CI) (CA INDEX NAME)

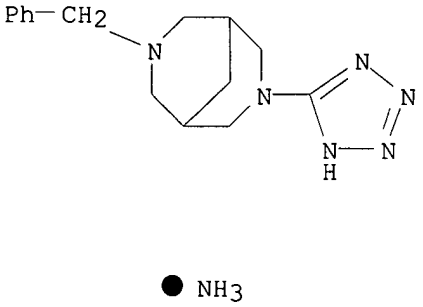


RN 389887-68-7 CAPLUS
CN Benzonitrile, 4-[[3-[7-(2-ethyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]amino]- (9CI) (CA INDEX NAME)



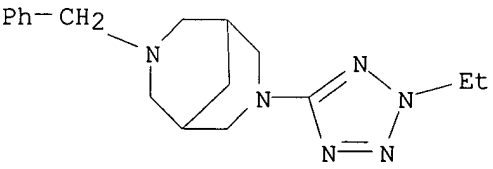
IT **389887-70-1P 389887-71-2P 389887-72-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of new bispidine compds. for the treatment of cardiac arrhythmias)

RN 389887-70-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)-7-(1H-tetrazol-5-yl)-, ammonium salt (9CI) (CA INDEX NAME)

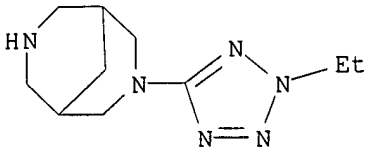


● $NH_3$

RN 389887-71-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-ethyl-2H-tetrazol-5-yl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 389887-72-3 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-ethyl-2H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



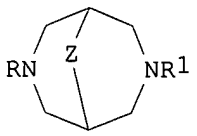
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:453062 CAPLUS
DOCUMENT NUMBER: 135:61360
TITLE: Preparation of heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands.
INVENTOR(S): Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Nielsen, Simon Feldbaek; Ahring, Philip K.; Jorgensen, Tino Dyhring
PATENT ASSIGNEE(S): Neurosearch A/S, Den.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001044243 | A2 | 20010621 | WO 2000-DK696 | 20001214 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DK 1999-1790 A 19991214
OTHER SOURCE(S): MARPAT 135:61360
GI



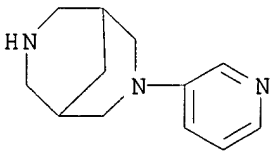
I

AB Title compds. [I; Z = (CH2)n; n = 0-2; R = H, alkyl, aryl, aralkyl,

fluorescent group; R1 = (substituted) mono- or polyheterocyclyl], were prepd. as drugs and diagnostic agents (no data). Thus, 3,7-dibenzyl-3,7-diazabicyclo[3.3.1]nonane (prepn. given) was stirred with HCO2H and Pd/C to give crude monobenzyl deriv., which was heated with 2-chloroquinoline at 100.degree. for 1 h to give 7-benzyl-3-(2-quinolinyl)-3,7-diazabicyclo[3.3.1]nonane. I may be useful for the treatment of central nervous system diseases, disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neurodegeneration inflammation, pain, and drug withdrawal symptoms.

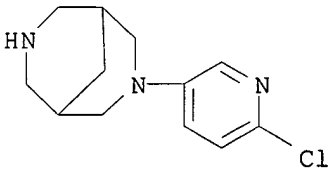
IT **286945-99-1P 286946-00-7P 286946-07-4P**
**345317-15-9P 345317-16-0P 345317-17-1P**
**345317-18-2P 345317-19-3P 345317-20-6P**
**345317-21-7P 345317-22-8P 345317-23-9P**
**345317-24-0P 345317-25-1P 345317-26-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands)

RN 286945-99-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)

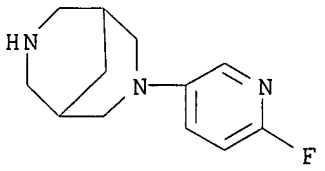



546/122
514/300

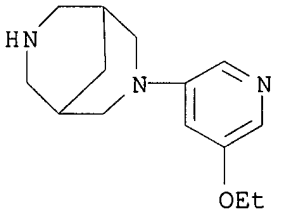
RN 286946-00-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



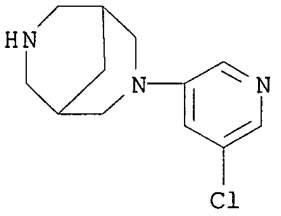

RN 286946-07-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



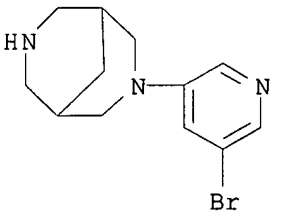
RN 345317-15-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 345317-16-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)

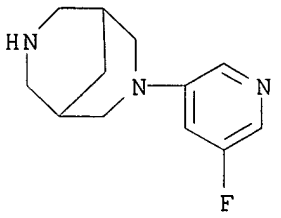


RN 345317-17-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-bromo-3-pyridinyl)- (9CI) (CA INDEX NAME)

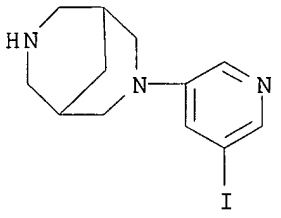


RN 345317-18-2 CAPLUS

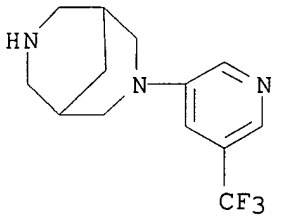
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



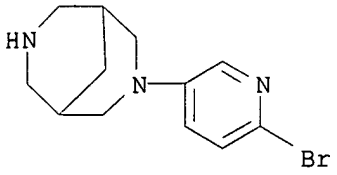
RN 345317-19-3 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)



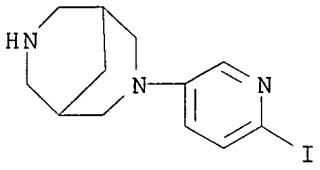
RN 345317-20-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[5-(trifluoromethyl)-3-pyridinyl]- (9CI) (CA INDEX NAME)



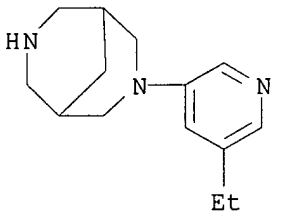
RN 345317-21-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-bromo-3-pyridinyl)- (9CI) (CA INDEX NAME)



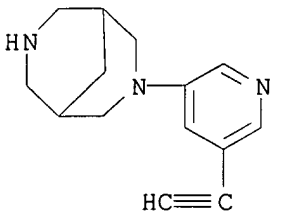
RN 345317-22-8 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 345317-23-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

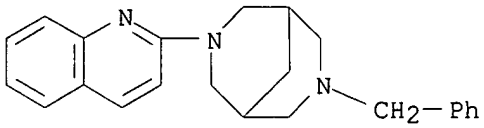


RN 345317-24-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethynyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

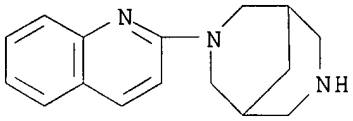


RN 345317-25-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)-7-(2-quinolinyl)- (9CI)

(CA INDEX NAME)



RN 345317-26-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-quinolinyl)- (9CI) (CA INDEX NAME)

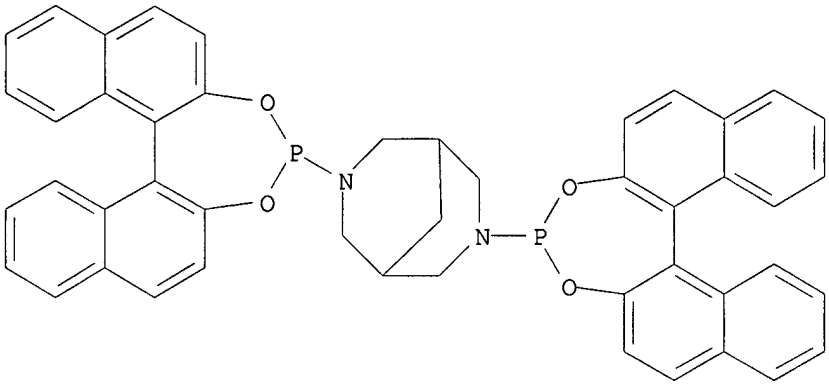


L8 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:120739 CAPLUS
DOCUMENT NUMBER: 134:326572
TITLE: Chiral bicyclic phosphoramidites - a new class of ligands for asymmetric catalysis
AUTHOR(S): Huttenloch, Oliver; Spieler, Jan; Waldmann, Herbert
CORPORATE SOURCE: Max-Planck-Institut fur molekulare Physiologie Abteilung Chemische Biologie, Dortmund, 44227, Germany
SOURCE: Chemistry--A European Journal (2001), 7(3), 671-675
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:326572

AB The development of new ligands for catalytic asym. C-C bond formation is of great interest to org. synthesis. The prepn. of new class of chiral phosphoramidites that embody one or two binaphthol units attached to an achiral azabicyclic [3.3.1] or [3.3.0] framework is described. These ligands were easily accessible from (R)-1,1'-binaphthyl-2,2'-dioxaphosphor-chloridite and the corresponding heterobicyclic core. They were employed in enantioselective Cu-catalyzed addns. of different dialkylzinc reagents to cyclic and acyclic enones. The chiral ketones were obtained with an enantiomeric ratio up to 91:9. The choice of the best ligand proved to be strongly dependent on each substrate. In addn., ligand derived from 1,5-dimethyl-3,7-diazabicyclo[3.3.0]octane was the most suitable for Rh-catalyzed hydrogenations of .alpha.,.beta.-unsatd. esters, giving rise to di-Me 2-methylsuccinate and Me N-acetylalaninate with enantiomer ratios up to 95:5.

IT **335616-63-2P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);

USES (Uses)
(prepn. of chiral bicyclic phosphoramidites as new class of ligands for
asym. catalysis)
RN 335616-63-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis[(11bR)-dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-yl]- (9CI) (CA INDEX NAME)



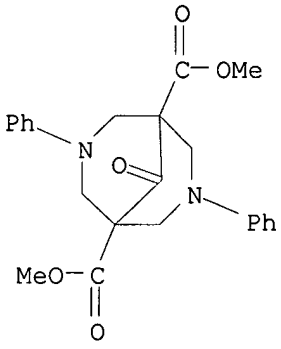
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:780169 CAPLUS
DOCUMENT NUMBER: 134:85911
TITLE: 1H NMR spectral study of some 4-hydroxy-2,6-diphenylpiperidines and a systematic analysis of 1H chemical shifts in some piperidines and 3,7-diazabicyclo[3.3.1]nonane derivatives
AUTHOR(S): Pandiarajan, K.; Manimekalai, A.; Rajarajan, G.
CORPORATE SOURCE: Department of Chemistry, Annamalai University, Annamalai Nagar, 608 002, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2000), 39B(7), 517-524
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1H NMR spectra have been recorded for some 3,5-dimethyl-2,6-diphenyl-4-piperidinol derivs. and their corresponding axial 4-hydroxy epimers. The proton chem. shifts and coupling consts. have been detd. by anal. of the spectra. The vicinal coupling consts. suggest that a boat form may make a slight contribution to the equatorial alcs. The .DELTA..delta.ea value for the protons in 5-position is less in the axial alc. than in the corresponding equatorial alc. and becomes neg. in one case. The effects

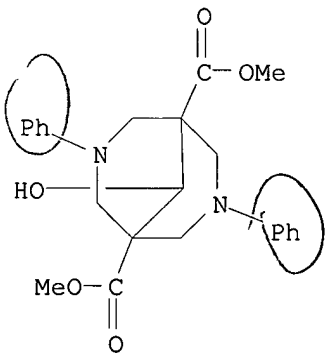
of Me, Et, iso-Pr and hydroxyl groups on the chem. shifts of the ring protons are discussed. Anal. of the chem. shifts of some 9-hydroxy-3,7-diazabicyclo[3.3.1]nonanes suggests that the 3,7-di-Ph substituted compds. exist in a boat-chair conformation.

IT **187521-32-0 187521-34-2 187800-56-2 317820-65-8**
RL: PRP (Properties)
(proton NMR study of some piperidinols and diazabicyclononane derivs.)

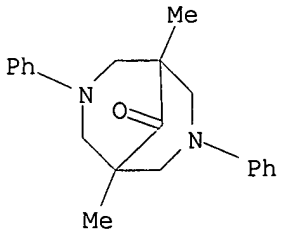
RN 187521-32-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)



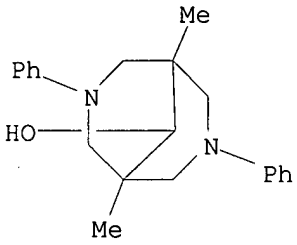

RN 187521-34-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-hydroxy-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)




RN 187800-56-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA INDEX NAME)




RN 317820-65-8 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:535147 CAPLUS
DOCUMENT NUMBER: 133:135332
TITLE: Preparation of diazabicyclic derivatives as nicotinic acetylcholine receptor ligands
INVENTOR(S): Bunnelle, William H.; Cristina, Daniela Barlocco; Daanen, Jerome F.; Dart, Michael J.; Meyer, Michael D.; Ryther, Keith B.; Schrimpf, Michael R.; Sippy, Kevin B.; Toupence, Richard B.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000044755 | A1 | 20000803 | WO 2000-US1620 | 20000125 |

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,

MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
EP 1147112 A1 20011024 EP 2000-906998 20000125
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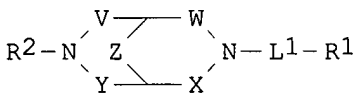
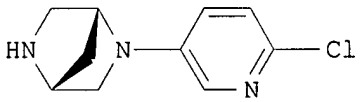
IE, SI, LT, LV, FI, RO
BR 2000007664 A 20020507 BR 2000-7664 20000125
NO 2001003731 A 20010918 NO 2001-3731 20010730
PRIORITY APPLN. INFO.: US 1999-239838 A 19990129
WO 2000-US1620 W 20000125
OTHER SOURCE(S): MARPAT 133:135332
GI




I



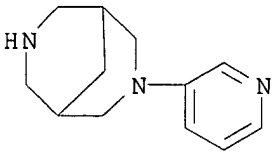

II

AB The title compds. (I) [wherein V and X = independently a bond or CH2; W and Y = independently a bond, CH2, or CH2CH2; Z = CH2, CH2CH2, or CH2CH2CH2; L1 = a bond or (CH2)n; n = 1-5; R1 = certain heteroarom. rings, such as pyridinyl, pyrimidinyl, pyrazinyl, quinolinyl, etc.; R2 = H, alkoxycarbonyl, (amino)alkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy(alkyl), phenoxycarbonyl, or NH2] and their pharmaceutically acceptable salts were prepd. as cholinergic modulators for the treatment of pain and other conditions. For example, (-)-II.bul.Ts-OH was prepd. in a multi-step sequence involving N-protection of (1R,4R)-2-benzyl-2,5-diazabicyclo[2.2.1]heptane.bul.2HBr with CO(OBu-t)2 (94%), debenzylation (93%), addn. of 2-chloro-5-iodopyridine (67%), and deprotection followed by salt formation (71%). (-)-II.bul.Ts-OH exhibited high affinity for the nicotinic acetylcholine receptor with Ki of 0.01 nM and showed a significant antinociceptive effect at the minimally ED of 0.62 .mu.mol/kg in the mouse hot plate paradigm.

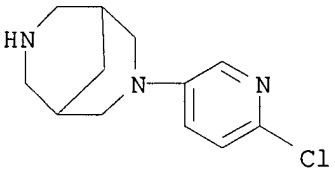
IT **286945-99-1P**, 3-(3-Pyridinyl)-3,7-diazabicyclo[3.3.1]nonane
**286946-00-7P**, 3-(6-Chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of N-substituted diazabicycloalkanes as nicotinic acetylcholine receptor ligands by addn. of haloheterocycles to protected diazabicyloalkanes followed by deprotection and optional substitution)

RN 286945-99-1 CAPLUS

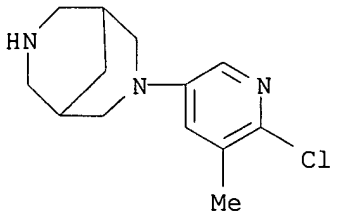
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)



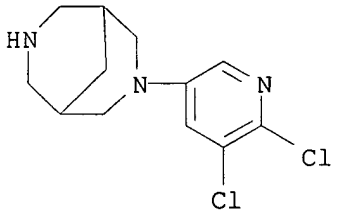
RN 286946-00-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



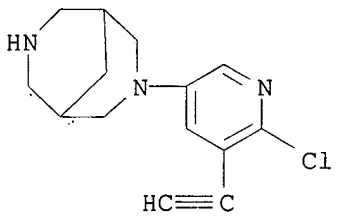
IT **286946-01-8P**, 3-(6-Chloro-5-methyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-02-9P**, 3-(5,6-Dichloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-03-0P**, 3-(6-Chloro-5-ethynyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-04-1P**, 3-(6-Chloro-5-cyano-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-05-2P**, 3-(5-Methoxy-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-06-3P**, 3-(6-Fluoro-5-methyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-07-4P**, 3-(6-Fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-08-5P**, 3-(5-Ethynyl-6-fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-09-6P**, 3-(5-Cyano-6-fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-10-9P**, 3-(5-Bromo-6-chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286947-18-0P**, 3-(3-Pyridinyl)-3,7-diazabicyclo[3.3.1]nonane bis(4-methylbenzenesulfonate) **286947-19-1P**, 3-(6-Chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane 4-methylbenzenesulfonate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-substituted diazabicycloalkanes as nicotinic acetylcholine receptor ligands by addn. of haloheterocycles to protected diazabicyloalkanes followed by deprotection and optional substitution)
RN 286946-01-8 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



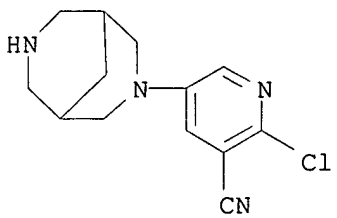
RN 286946-02-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5,6-dichloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



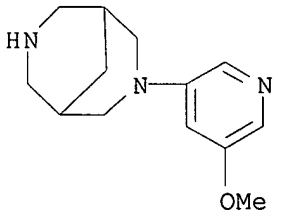
RN 286946-03-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-ethynyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



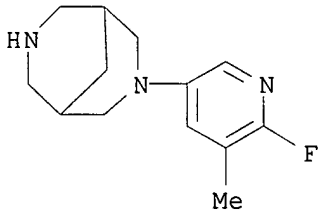
RN 286946-04-1 CAPLUS
CN 3-Pyridinecarbonitrile, 2-chloro-5-(3,7-diazabicyclo[3.3.1]non-3-yl)- (9CI) (CA INDEX NAME)



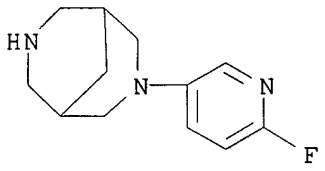
RN 286946-05-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



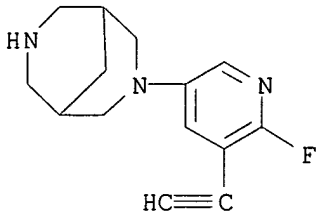

RN 286946-06-3 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-5-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



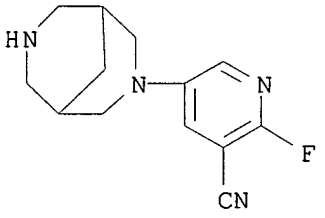

RN 286946-07-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



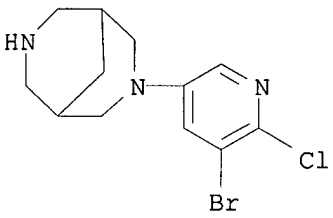

RN 286946-08-5 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethynyl-6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 286946-09-6 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(3,7-diazabicyclo[3.3.1]non-3-yl)-2-fluoro- (9CI) (CA INDEX NAME)



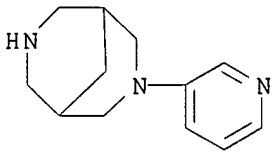
RN 286946-10-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-bromo-6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 286947-18-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

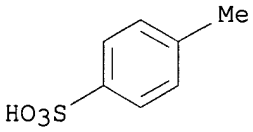
CM 1

CRN 286945-99-1
CMF C12 H17 N3



CM 2

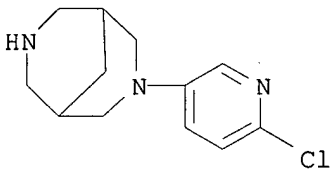
CRN 104-15-4
CMF C7 H8 O3 S



RN 286947-19-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

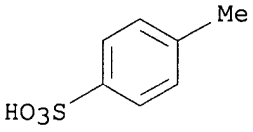
CM 1

CRN 286946-00-7
CMF C12 H16 Cl N3



CM 2

CRN 104-15-4
CMF C7 H8 O3 S



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

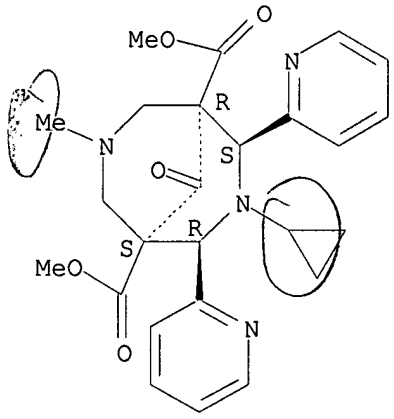
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:531065 CAPLUS
DOCUMENT NUMBER: 133:232367
TITLE: Diazabicyclo[3.3.1]nonanone-type ligands for the opioid receptors
AUTHOR(S): Kuhl, Ulrich; Englberger, Werner; Haurand, Michael; Holzgrabe, Ulrike
CORPORATE SOURCE: Institut fur Pharmazie und Lebensmittelchemie, Universitat Wurzburg, Wurzburg, D-97074, Germany
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(7), 226-230
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Previously 2,4-dipyridine substituted 3,7-diazabicyclo-[3.3.1]nonanone diesters were found to have a high affinity and selectivity towards the .kappa.-opioid receptor. The purpose of this study was to check the influence of substituents at position N3 on the affinity to the .mu.-, .delta.-, and .kappa.-receptors. Whereas a phenylethyl group is able to create affinity to the .mu.-receptor, small substituents such as a hydrogen or a Me group are responsible for a high affinity to the .kappa.-receptor. In addn., a dimeric compd. was found to have affinity to the .kappa.-receptor. Although all compds. will bear at least one pos.
charge under physiol. conditions they show a considerable lipophilicity, indicating the possibility of passing the blood-brain barrier.

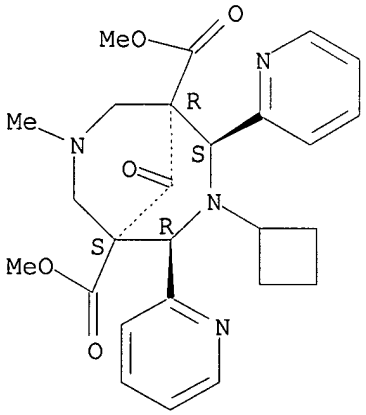
IT **294181-79-6 294181-83-2 294181-86-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); PRP (Properties); BIOL (Biological study)
(diazabicyclononanone-type ligands for opioid receptors)
RN 294181-79-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 3-cyclopropyl-7-methyl-9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (1R,2S,4R,5S)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



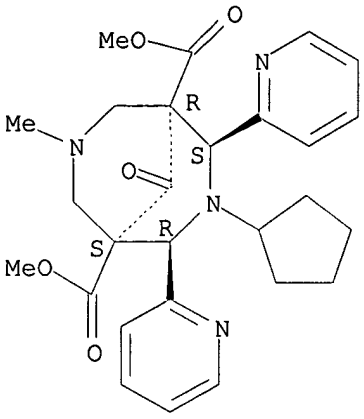
RN 294181-83-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 3-cyclobutyl-7-methyl-9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (1R,2S,4R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 294181-86-5 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 3-cyclopentyl-7-methyl-9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (1R,2S,4R,5S)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



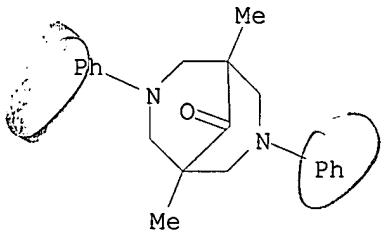

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:694267 CAPLUS
DOCUMENT NUMBER: 130:66587
TITLE: Conformational Restriction of Acyclic .pi.-Allyl Ligands in (3,7-Diphenyl-1,5-dimethylbispidinone)(.eta.3-alkenyl)palladium Complexes
AUTHOR(S): Gogoll, Adolf; Grennberg, Helena; Axen, Andreas
CORPORATE SOURCE: Department of Organic Chemistry, University of Uppsala, Uppsala, 751 21, Swed.
SOURCE: Organometallics (1998), 17(24), 5248-5253
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A chelating dinitrogen ligand based on the bispidine skeleton is shown to restrict the conformational freedom of small, acyclic .pi.-allyl ligands in Pd complexes. The .pi.-allyl ligand is locked into one single rotamer by entirely steric interactions. These interactions do not require the presence of bulky substituents on the .pi.-allyl ligand. The geometry of these complexes was studied by NMR spectroscopy in combination with semiempirical calcns.

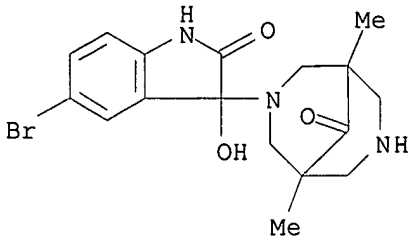
IT **187800-56-2**, 3,7-Diphenyl-1,5-dimethylbispidinone
RL: RCT (Reactant); RACT (Reactant or reagent)
(conformational restriction of acyclic .pi.-allyl ligands in (diphenyldimethylbispidinone)(.eta.3-alkenyl)palladium complexes)

RN 187800-56-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA INDEX NAME)

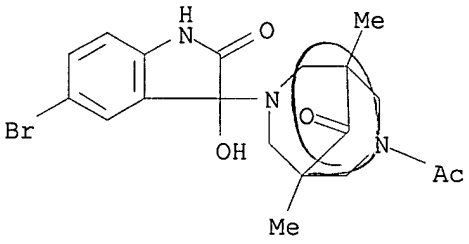



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:484412 CAPLUS
DOCUMENT NUMBER: 129:189250
TITLE: Synthesis and conversions of polyhedral compounds. 25.
Synthesis and conversions of certain oxindole derivatives of 1,3-diazaadamantane and 3,7-diazabicyclo[3.3.1]nonane
AUTHOR(S): Agadzhanyan, Ts. E.; Gevorkyan, K. A.
CORPORATE SOURCE: A. L. Mndzhoyan Institute of Fine Organic Chemistry, Academy of Sciences of the Republic of Armenia, Yerevan, 375014, Armenia
SOURCE: Chemistry of Heterocyclic Compounds (New York)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1998), Volume Date 1997, 33(11), 1288-1291
CODEN: CHCCAL; ISSN: 0009-3122
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
AB By the reaction of 1,5-dimethyl-9-oxo-3,7-diazabicyclo[3.3.1]nonane with isatin and a no. of its derivs., spiro(1,3-diazaadamantane-2,3'-oxindoles) have been synthesized. In the case of 5-bromoisatin, either 3-(3-hydroxyoxindolyl)-3,7-diazabicyclo[3.3.1]nonane or the corresponding spirane is obtained, depending on the temp. The interaction of these products with acetic anhydride has been studied.
IT **211917-31-6P 211917-33-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactions of diazabicyclononane with isatins)
RN 211917-31-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-(5-bromo-2,3-dihydro-3-hydroxy-2-oxo-1H-indol-3-yl)-1,5-dimethyl- (9CI) (CA INDEX NAME)



RN 211917-33-8 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-acetyl-7-(5-bromo-2,3-dihydro-3-hydroxy-2-oxo-1H-indol-3-yl)-1,5-dimethyl- (9CI) (CA INDEX NAME)

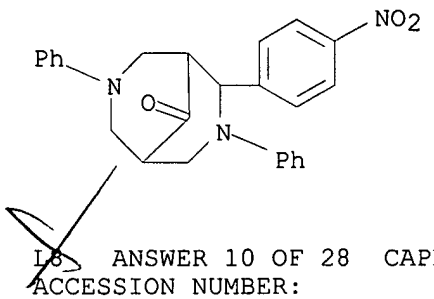


L8 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:665555 CAPLUS
DOCUMENT NUMBER: 127:307286
TITLE: Study on the synthesis and antibacterial activity of mannich bases containing .alpha.,.beta.-unsaturated ketone
AUTHOR(S): Gu, Shangxiang; Yao, Kaling; Gu, Yonghong
CORPORATE SOURCE: Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
SOURCE: Yaoxue Xuebao (1997), 32(1), 38-42
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB 12 Mannich bases contg. .alpha.,.beta.-unsatd. ketone were synthesized and characterized by elemental anal., IR, 1HNMR, UV and MS spectra. Some of the compds. showed marked antibacterial activity.

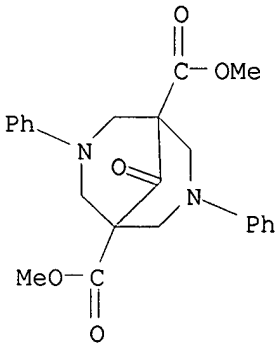
IT **197514-66-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(study on the synthesis and antibacterial activity of mannich bases

contg. .alpha.,.beta.-unsatd. ketone)
RN 197514-66-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2-(4-nitrophenyl)-3,7-diphenyl- (9CI) (CA INDEX NAME)

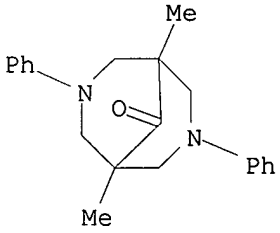



L8 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:172468 CAPLUS
DOCUMENT NUMBER: 126:199654
TITLE: (.pi.-Allyl)palladium Complexes with N,N'-Diphenylbispidinone Derivatives as a New Type of Chelating Nitrogen Ligand: Complexation Studies, Spectroscopic Properties, and an X-ray Structure of (3,7-Diphenyl-1,5-dimethylbispidinone)[(1,3-.eta.3-propenyl)-palladium] Trifluoromethanesulfonate
AUTHOR(S): Gogoll, Adolf; Grennberg, Helena; Axen, Andreas
CORPORATE SOURCE: Department of Organic Chemistry, University of Uppsala, Uppsala, 751 21, Swed.
SOURCE: Organometallics (1997), 16(6), 1167-1178
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:199654
AB A series of 3,7-diazabicyclo[3.3.1]nonane (bispidine) derivs. have been synthesized, and their properties as bidentate nitrogen ligands for (.pi.-allyl)palladium complexes have been investigated. Complexes of these ligands and of N,N'-diphenylpiperazine and N,N'-diphenyl-1,4-diazacyclooctane with (1,3-.eta.3-propenyl)palladium are described, in particular their effects on the proton chem. shifts of the .pi.-allyl ligand. Ligand dynamics of the complexes is discussed. The structure of [(3,7-diphenyl-1,5-dimethylbispidinone)(1,3-.eta.3-propenyl)Pd]CF3SO3 has been detd. by x-ray crystallog. N,N'-Diphenylbispidine derivs. show an unusually large steric interaction with the .pi.-allyl ligand, indicated by a tilt of the .pi.-allyl plane toward the N-Pd-N plane by 122.8(8).degree.. Chem. shift changes of the .pi.-allyl protons due to the arom. ring current are related to the geometry of the complexes. The ligands are tested on the larger 2-methylene-6,6-dimethylbicyclo[3.1.1]hept-2,3,10-.eta.3-enyl ligand, demonstrating their potential as chem. shift reagents.
IT **187521-32-0P 187800-56-2P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of allylpalladium complexes with diphenylbispidinone derivs. as
new type of chelating nitrogen ligand and their complexation studies

and spectroscopic properties)
RN 187521-32-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)



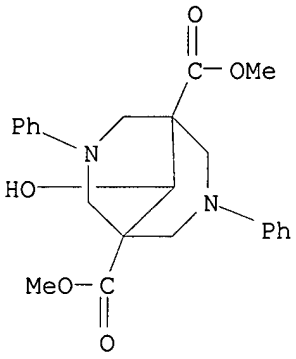
RN 187800-56-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA INDEX NAME)



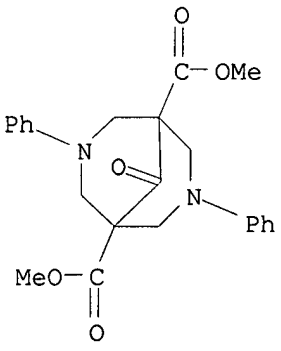
L8 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:57952 CAPLUS
DOCUMENT NUMBER: 126:185747
TITLE: Chemical shift assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes: an unexpected deviation from the axial/equatorial chemical shift order
AUTHOR(S): Gogoll, Adolf; Grennberg, Helena; Axen, Andreas
CORPORATE SOURCE: Department of Organic Chemistry, University of Uppsala, Uppsala, 751 21, Swed.
SOURCE: Magnetic Resonance in Chemistry (1997), 35(1), 13-20
CODEN: MRCHEG; ISSN: 0749-1581
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The chem. shift order of axial and equatorial methylene protons in 1,5-disubstituted 3,7-diazabicyclo [3.3.1] nonan-9-ones may be altered by substituents in the 1,5-positions, but the corresponding alcs. behave differently. Unambiguous signal assignments for a series of the title

compds. are provided, based on 3JCH coupling consts. and on {1H} 13C heteronuclear Overhauser effects. Substituent anisotropy effects as a source of the chem. shift changes are discussed.

IT **187521-34-2P**
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(deviation from axial/equatorial chem. shift order and chem. shift assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes)
RN 187521-34-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-hydroxy-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)

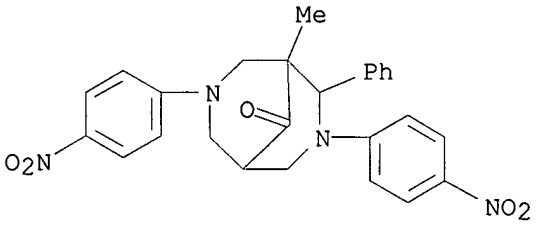



IT **187521-32-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(deviation from axial/equatorial chem. shift order and chem. shift assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes)
RN 187521-32-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)




L8 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:322870 CAPLUS
DOCUMENT NUMBER: 120:322870
TITLE: Mannich reaction with arylamine as the amino

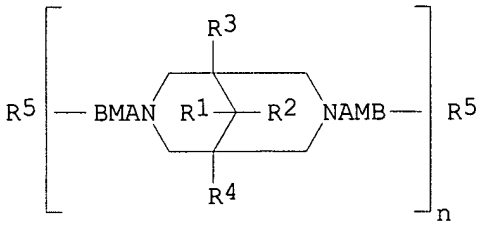
component. (X). Mannich reaction of arylamine with benzylidenebutanone
AUTHOR(S): Liao, Hongbiao; Li, Yan; Xu, Xiujuan
CORPORATE SOURCE: Dep. Chem., Beijing Normal Univ., Beijing, 100875, Peop. Rep. China
SOURCE: Beijing Shifan Daxue Xuebao, Ziran Kexueban (1992), 28(3), 367-71
CODEN: BSDKDH; ISSN: 0476-0301
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Mannich reaction of PhCH:CR1COCH2R2 (R1, R2 = H, Me) with R3NH2 (R3 = Ph, 4-ClC6H4, 4-BrC6H4, 3,4-Cl2C6H3, 4-MeC6H4, 4-MeOC6H4, 4-methoxy-2-nitrophenyl) gave 60-85% PhCH:CR1COCHR2CH2NHR3.
IT **155498-59-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 155498-59-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-3,7-bis(4-nitrophenyl)-2-phenyl- (9CI) (CA INDEX NAME)




L8 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:118865 CAPLUS
DOCUMENT NUMBER: 112:118865
TITLE: Preparation of 3,7-diazabicyclo[3.3.1]nonanes as heat and light stabilizers
INVENTOR(S): Aumueller, Alexander; Neumann, Peter; Trauth, Hubert
PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

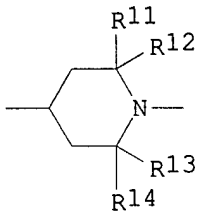
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 3743279 | A1 | 19890629 | DE 1987-3743279 | 19871219 |
| US 4943391 | A | 19900724 | US 1988-286295 | 19881210 |
| EP 324945 | A2 | 19890726 | EP 1988-120776 | 19881213 |
| EP 324945 | A3 | 19910116 | | |
| EP 324945 | B1 | 19940309 | | |
| R: BE, CH, DE, FR, GB, IT, LI | | | | |
| JP 01211588 | A2 | 19890824 | JP 1988-318709 | 19881219 |

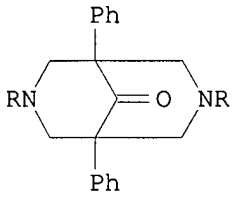
PRIORITY APPLN. INFO.: DE 1987-3743279 19871219
OTHER SOURCE(S): CASREACT 112:118865
GI




I

Q=



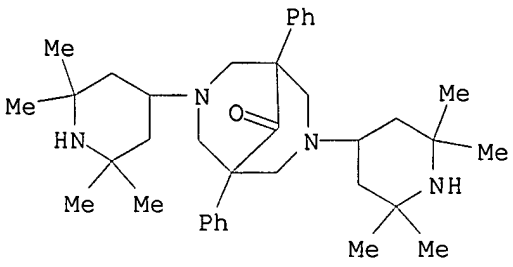

II

AB The title compds. [I; A, B = bond, C1-22 alkylene, cycloalkylene, (CH2)mO2, (CH2)mCONR10, (CH2)mCONH(CH2)l; M = piperidinediyl group Q which may be bound to A via the C- or N-atom; R1 = H, R2 = H, OH; R1R2 = O; R3, R4 = (un)substituted Ph, 1- or 2-naphthyl; R5 = H, cyano, OH, alkanoyloxy, etc.; MBR5 = substituted hydroxyphenyl, N-attached heterocyclyl; R10 = H, C1-22 alkyl, Ph, etc.; R11-R14 = C1-4 alkyl; R11R12, R13R14 = (CH2)4-5; l, m = 1-20; n = 1-70] were prepd. as heat and light stabilizers for org. materials (no data). Thus, (PhCH2)2CO, QH2(R11-R14 = Me), and paraformaldehyde were heated 6 h in EtOH to give title compd. II (R = C-attached QH, R11-R14 = Me).

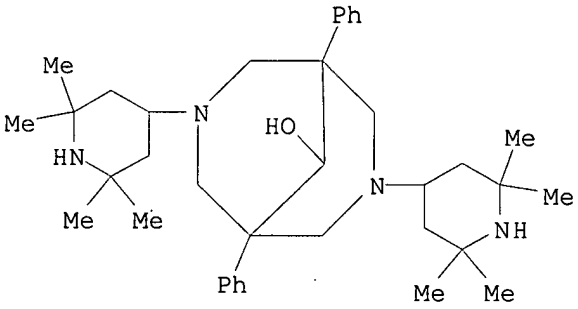
IT **124699-37-2P 124699-38-3P 124699-39-4P**
**124699-40-7P 124699-41-8P 125636-30-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as heat and light stabilizer)

RN 124699-37-2 CAPLUS

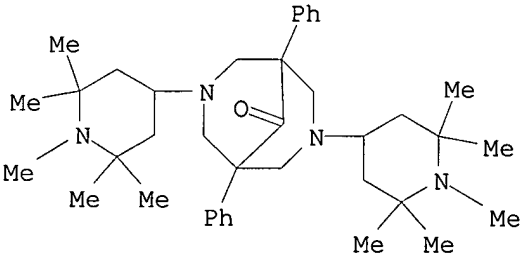
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-diphenyl-3,7-bis(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)



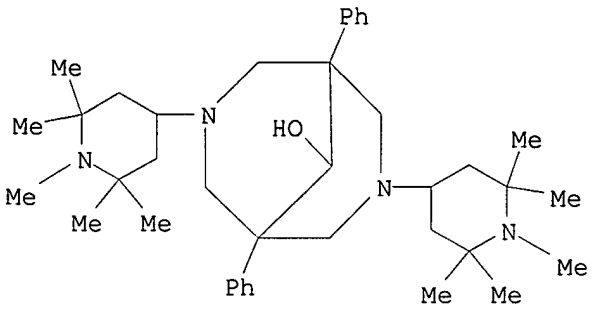
RN 124699-38-3 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 1,5-diphenyl-3,7-bis(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)



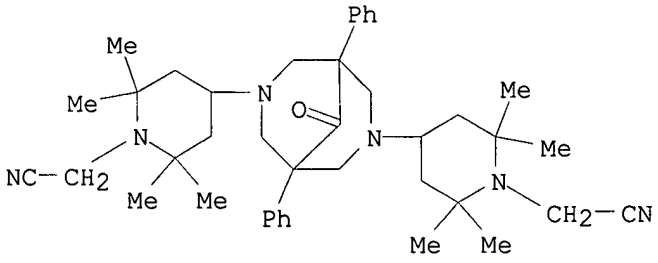
RN 124699-39-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-1,5-diphenyl- (9CI) (CA INDEX NAME)



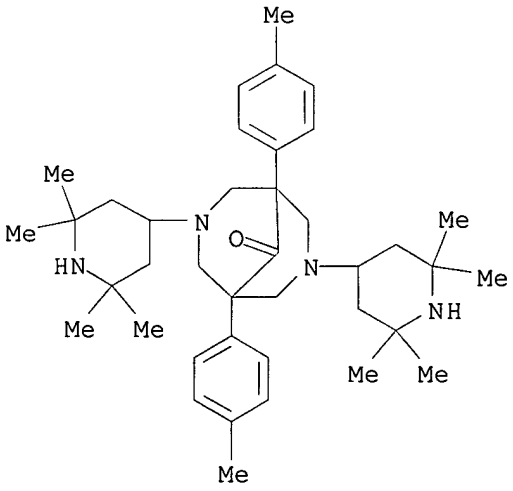
RN 124699-40-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 3,7-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-1,5-diphenyl- (9CI) (CA INDEX NAME)



RN 124699-41-8 CAPLUS
CN 1-Piperidineacetonitrile, 4,4'-(9-oxo-1,5-diphenyl-3,7-diazabicyclo[3.3.1]nonane-3,7-diyl)bis[2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



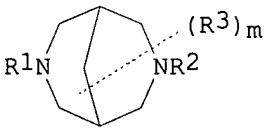
RN 125636-30-8 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-bis(4-methylphenyl)-3,7-bis(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:415252 CAPLUS
DOCUMENT NUMBER: 111:15252
TITLE: Improving the lightfastness of colored organic materials
INVENTOR(S): Kaneko, Yutaka
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 63281158 | A2 | 19881117 | JP 1987-116326 | 19870513 |

GI

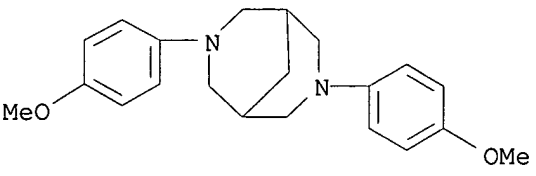



I

AB In the title method, an org. colored material and I [R1, R2 = H, alkyl, cycloalkyl, alkenyl, cycloalkenyl, alkynl, aryl, heterocycycl, acyl, sulfonyl, carbamoyl, phosphonyl, sulfamoyl, oxycarbonyl; R3 = substituent; m = 0-6] are allowed to coexist. The method is esp. useful in color photog., inks and fabric dyes. A photog material contained I [R1 = CH3; R2 = C6H5CH2] and a magenta dye to prevent photofading.

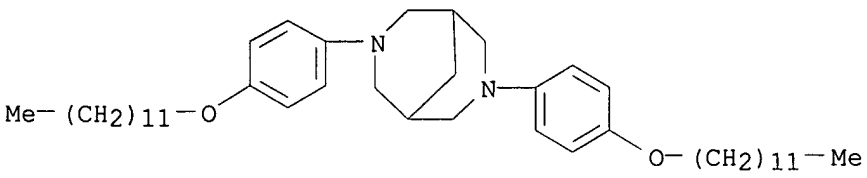
IT **121171-68-4 121171-69-5 121171-70-8 121171-72-0 121171-73-1 121171-76-4 121185-53-3**
RL: USES (Uses)
(lightfastness improvement additive, for orgs.)

RN 121171-68-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

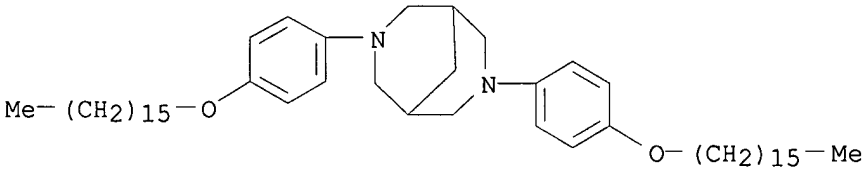



RN 121171-69-5 CAPLUS

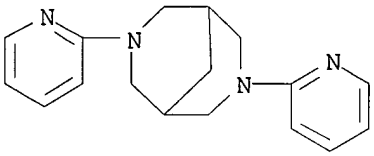
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis[4-(dodecyloxy)phenyl]- (9CI) (CA INDEX NAME)



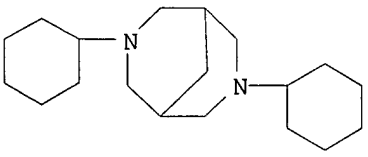
RN 121171-70-8 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis[4-(hexadecyloxy)phenyl]- (9CI) (CA INDEX NAME)



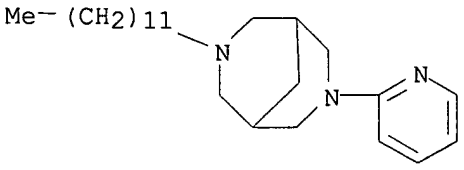
RN 121171-72-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-di-2-pyridinyl- (9CI) (CA INDEX NAME)



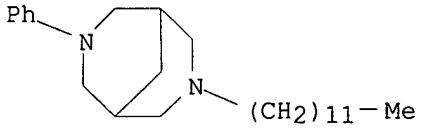
RN 121171-73-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-dicyclohexyl- (9CI) (CA INDEX NAME)



RN 121171-76-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-dodecyl-7-(2-pyridinyl)- (9CI) (CA INDEX NAME)



RN 121185-53-3 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-dodecyl-7-phenyl- (9CI) (CA INDEX NAME)



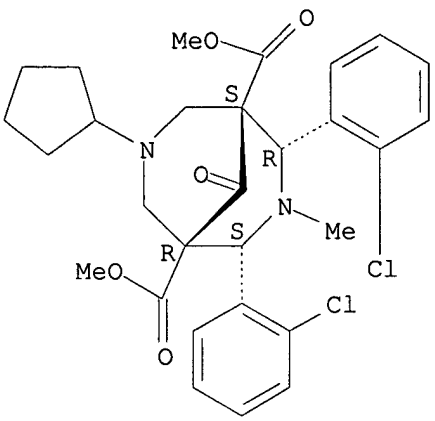
L8 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:470647 CAPLUS
DOCUMENT NUMBER: 103:70647
TITLE: Synthesis and conformational study of 3,7-diazabicyclo[3.3.1]nonan-9-ones
AUTHOR(S): Caujolle, Raymond; Castera, Pierre; Lattes, Armand
CORPORATE SOURCE: Lab. Chim. Ther., Toulouse, 31077, Fr.
SOURCE: Bull. Soc. Chim. Fr. (1984), (9-10, Pt. 2), 413-16
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French

AB 1H and 13C NMR studies of various 3,7-diazabicyclo [3.3.1]nonanones indicate an equil. between chair-chair and chair-boat conformations for these compds. N(7) atom bears bulky substituents, the chair-boat form is more favored at equil.

IT **97564-84-6 97564-85-7 97564-86-8 97564-87-9 97564-89-1**
RL: PRP (Properties)
(carbon-13 and proton NMR of, conformation in relation to)

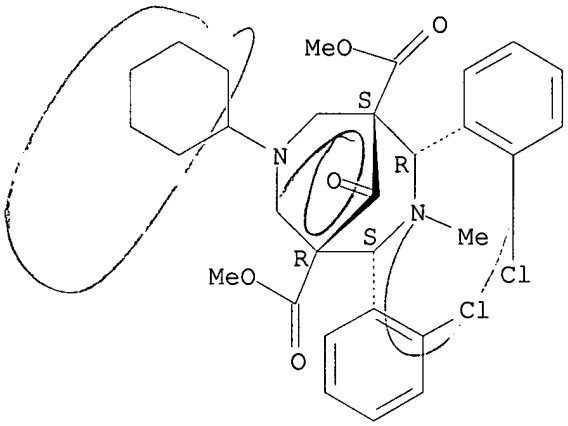
RN 97564-84-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-7-cyclopentyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



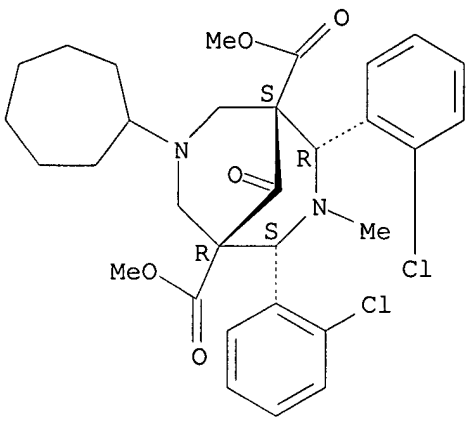

RN 97564-85-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-7-cyclohexyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



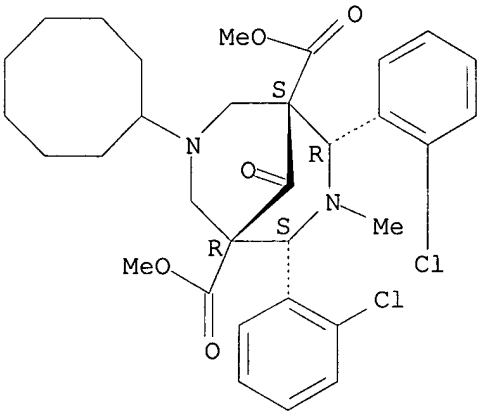

RN 97564-86-8 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-7-cycloheptyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

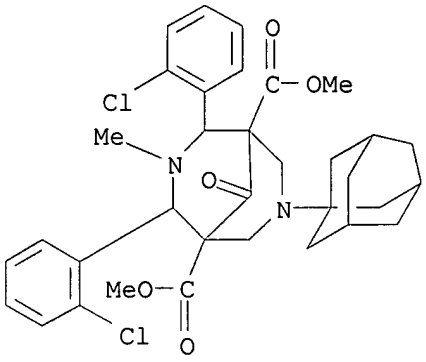



RN 97564-87-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-7-cyclooctyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)- (9CI) (CA INDEX NAME)

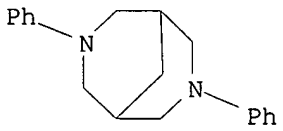
Relative stereochemistry.




RN 97564-89-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-3-methyl-9-oxo-7-tricyclo[3.3.1.13,7]dec-1-yl-, dimethyl ester, (endo,endo)- (9CI) (CA INDEX NAME)



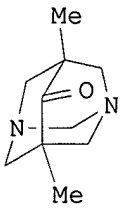
L8 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:581621 CAPLUS
DOCUMENT NUMBER: 101:181621
TITLE: Crystal and molecular structure of 3,7-diphenyl-3,7-diazabicyclo[3.3.1]nonane, C19H22N2
AUTHOR(S): Levina, O. I.; Potekhin, K. A.; Kurkutova, E. N.; Struchkov, Yu. T.; Palyulin, V. A.; Zefirov, N. S.
CORPORATE SOURCE: Vladimir. Pedagog. Inst., Vladimir, USSR
SOURCE: Dokl. Akad. Nauk SSSR (1984), 277(2), 367-70 [Crystallogr.]
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The title compd. is monoclinic, space group P21/c, with a 10.060(1), b 17.338(2), c 9.123(2) .ANG., and .beta. 100.62(1).degree.; Z = 4. The at.
parameters are given. The structure was detd. by direct methods and refined by full-matrix least-squares to R = 0.074. The mol. has the double-chain conformation.
IT **54171-89-0**
RL: PRP (Properties)
(structure of)
RN 54171-89-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)



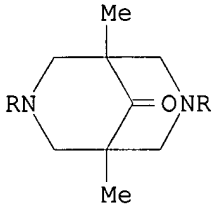
L8 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:104172 CAPLUS
DOCUMENT NUMBER: 96:104172
TITLE: Synthesis and reactions of polyhedral compounds. II.

Synthesis of 5,7-dimethyl-1,3-diazaadamantan-6-one and
-6-ol and their conversion into 3,7-diacyl(dicarbalkoxy, diarylsulfonyl)-3,7-diazabicyclo[3,3,1]nonanes

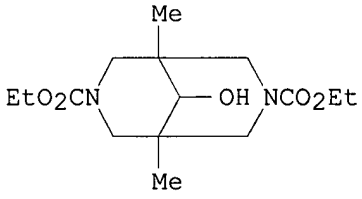
AUTHOR(S): Agadzhanyan, Ts. E.; Arutyunyan, G. L.
CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SOURCE: Arm. Khim. Zh. (1981), 34(11), 963-8
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I



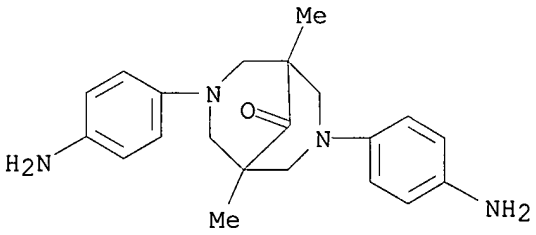
II



III

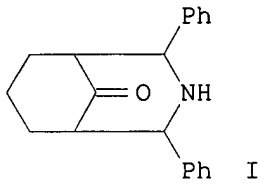
AB Cyclocondensation of EtCOEt, HCHO, and AcONH4 gave 19.5% I, which reacted with RCOCl, RO2CCl, or ArSO2Cl to give II [R = BrCH2CO, BrCH2CH2CO, CH2:CHCO, Bz, (phthalimidomethoxy)carbonyl, EtOCO, PhCH2OCO, 4-MeC6H4SO2, 4-(MeO2CNH)C6H4SO2]. LiAlH4 redn. of I gave 83.3% alc., which with ClCO2Et gave III.

IT **80808-97-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 80808-97-5 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(4-aminophenyl)-1,5-dimethyl- (9CI) (CA INDEX NAME)

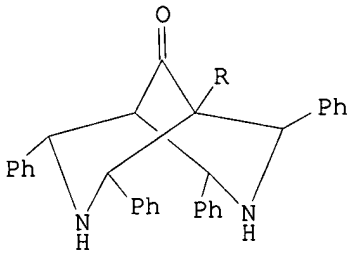



L8 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:425025 CAPLUS
DOCUMENT NUMBER: 95:25025
TITLE: Synthesis and reactions of ketones of 3-aza-, 3,7-diazabicyclononane and 3,7-diazaadamantane series

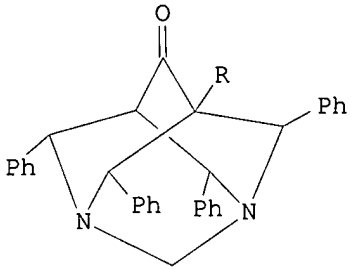
AUTHOR(S): Omarov, T. T.; Baisalbaeva, S. A.; Gubasheva, A. Sh.
CORPORATE SOURCE: USSR
SOURCE: Tr. Inst. Khim. Nauk, Akad. Nauk Kaz. SSR (1980), 52, 147-70
CODEN: TIKNAG; ISSN: 0568-5087
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I



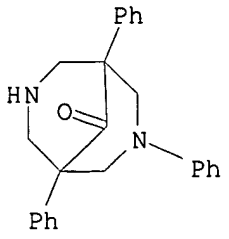
II



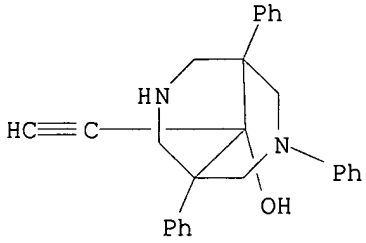
III

AB Condensation of cyclohexanone with BzH and H4NOAc gave a mixt. of diazabicyclononanone I and 2,6-dibenzylidenecyclohexanone. I was methylated. The diazabicyclononanes II (R = H, Me) were obtained by a similar condensation from the resp. piperidinone. The diazaadamantanes III were obtained from II by condensation with HCHO. III were reduced to alcs. I was converted to acetylenic alcs. Addnl. reactions of I, II and III were discussed. The conformation, spectra and biol. activity of I, II and III were discussed with 72 refs.

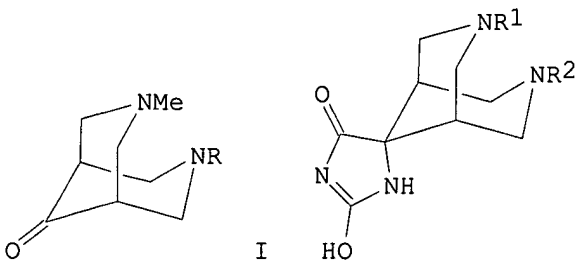
IT **77446-47-0P 77446-50-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)
RN 77446-47-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,3,5-triphenyl- (9CI) (CA INDEX NAME)



RN 77446-50-5 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 9-ethynyl-1,3,5-triphenyl- (9CI) (CA INDEX NAME)



L8 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:426411 CAPLUS
DOCUMENT NUMBER: 93:26411
TITLE: Spiro heterocyclic derivatives. XV. Some N-methyl-N'-alkyl(or aralkyl)-3,7-diazabicyclo[3.3.1]nonan-9-ones and some 9-spiro-5'-hydantoin derivatives of 3,7-diazabicyclo[3.3.1]nonanes
AUTHOR(S): Gonzalez Trigo, G.; Galvez Ruano, E.; Menendez Aguirre, C.
CORPORATE SOURCE: Fac. Farm., Univ. Complutense Madrid, Madrid, Spain
SOURCE: An. Quim. (1979), 75(12), 894-8
CODEN: ANQUBU; ISSN: 0365-4990
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
GI

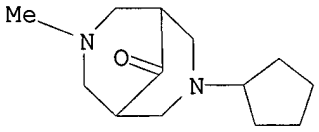


I II

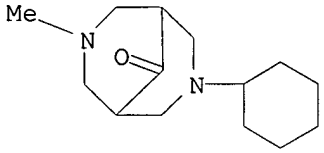
AB Reaction of N-methyl-4-piperidone with HCHO and amines RNH2 in AcOH soln. gave the 3,7-diazabicyclo[3.3.1]nonan-9-ones I [R = C1-C4 alkyl, cyclopentyl, cyclohexyl, PhCH2, PhCH2CH2, Me2N(CH2)3, HOCH2CH2], which reacted with KCN and (NH4)2CO3 to give the spirohydantoins II (R1 = Me, R2
= R or R1 = R, R2 = Me). IR band of I and II and NMR chem. shifts of II are tabulated.

IT **73977-30-7P 73990-91-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and IR spectrum of)

RN 73977-30-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclopentyl-7-methyl- (9CI) (CA INDEX NAME)

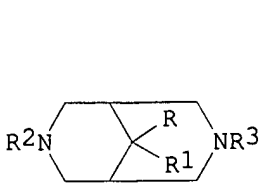



RN 73990-91-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclohexyl-7-methyl- (9CI) (CA INDEX NAME)

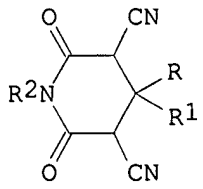



L8 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2002 ACS

| | |
|---|---|
| ACCESSION NUMBER: | 1977:601499 CAPLUS |
| DOCUMENT NUMBER: | 87:201499 |
| TITLE: | Nonsymmetric N-substituted bispidine (3,7-diazabicyclo[3.3.1]nonane. I |
| AUTHOR(S): | Hoerlein, Ulrich |
| CORPORATE SOURCE: | Chem. Wiss. Lab. Pharma, Bayer A.-G., Wuppertal, Ger. |
| SOURCE: | Eur. J. Med. Chem. - Chim. Ther. (1977), 12(4), 301-5 CODEN: EJMCA5 |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | German |
| GI | |




I




II

AB Bispidine derivs. I [R = R1 = Me, RR1 = (CH2)5, R2 = Me, Et, CH2Ph, R3 = H; RR1 = (CH2)4, R2 = Me, Et, R3 = H] were prepd. by condensing RR1C:C(CN)CO2Et with R2NHCOCH2CN, hydrolyzing II, and reducing diimides with LiAlH4. I [R3 = acyl, 4-FC6H4CO(CH2)3, 8-chloro-10,11-dihydrobenzo[b,f]thiepin-10-yl] were prepd. by substitution of I (R3 = H).

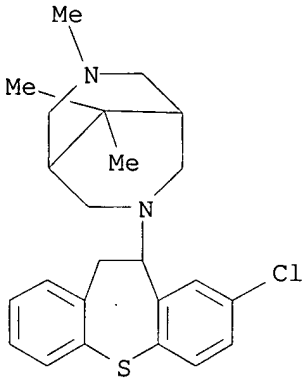
I [RR1 = (CH2)5, (CH2)4, R2 = Me, R3 = COCH2Ph] had analgesic activities of the same magnitude as morphine. Some other I exhibited various pharmacol. activity, but only to a degree.

IT **64729-96-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 64729-96-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(8-chloro-10,11-dihydrodibenzo[b,f]thiepin-10-yl)-7,9,9-trimethyl- (9CI) (CA INDEX NAME)




L8 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:484859 CAPLUS

DOCUMENT NUMBER: 87:84859

TITLE: Synthesis of 4,9-diheterotricyclo[4.4.0.02,7]decanes and bicyclo[3.3.1]nonanes

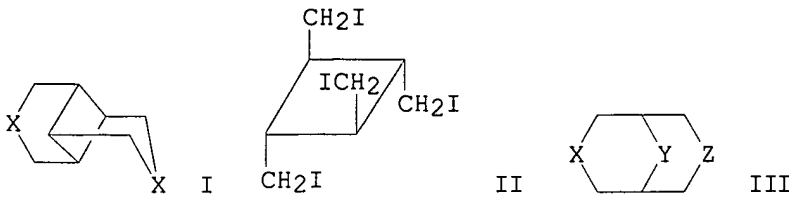
AUTHOR(S): Zefirov, N. S.; Rogozina, S. V.

CORPORATE SOURCE: Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR

SOURCE: Strukt. Svoistva Krist. (1974), 1, 94-9
CODEN: SSKRDM

DOCUMENT TYPE: Journal

LANGUAGE: Russian
GI



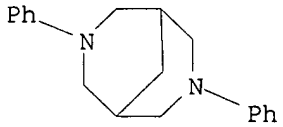

I II III

AB Tricyclodecane I (X = S) was obtained in 60% yield by refluxing II with Na2S in abs. alc. 6 h. Analogously II refluxed with PhNH2 60 h in PhMe gave I (X = NPh). Bicyclononanes III (X = O, Y = O, S, Z = S; X = S, Y = O, Z = S, Se) were obtained in 1.0-18.8% yields by treatment of a bis(iodomethyl)dioxane, oxathiane with Na2S or with Se. Addnl. obtained was 73.7% III (X = Z = NPh, Y = CH2).

IT **54171-89-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 54171-89-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)




L8 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2002 ACS

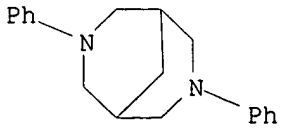
ACCESSION NUMBER: 1976:90040 CAPLUS
DOCUMENT NUMBER: 84:90040
TITLE: Synthesis of 4,9-diheterotricyclo[4.4.0.02,7]decanes and bicyclo[3.3.1]nonanes
AUTHOR(S): Zefirov, N. S.; Rogozina, S. V.
CORPORATE SOURCE: USSR
SOURCE: Struktura I Svoistva Kristallov (1974), (1), 94-9
From: Ref. Zh., Khim. 1975, Abstr. No. 19ZH312
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Title only translated.

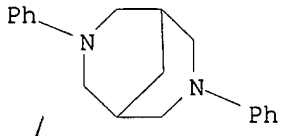
IT **54171-89-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 54171-89-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)

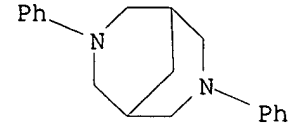


L8 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:52620 CAPLUS
DOCUMENT NUMBER: 84:52620
TITLE: Crystallographic data of the compounds, N,N-diphenyl-3,7-diazabicyclo[3,3,1]nonane (C19H22N2) and C22H20N2O2
AUTHOR(S): Levina, O. I.
CORPORATE SOURCE: USSR
SOURCE: Struktura I Svoistva Kristallov (1974), (1), 112-13
From: Ref. Zh., Khim. 1975, Abstr. No. 15B544
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Title only translated.
IT **54171-89-0**
RL: PRP (Properties)
(crystal structure of)
RN 54171-89-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)

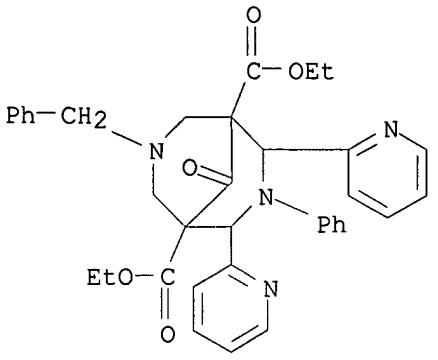


L8 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:57412 CAPLUS
DOCUMENT NUMBER: 82:57412
TITLE: Stereochemical studies. XVIII. Conformational study of heteroanalogs of bicyclo[3.3.1]nonane
AUTHOR(S): Zefirov, N. S.; Rogozina, S. V.
CORPORATE SOURCE: Chem. Dep., Moscow State Univ., Moscow, USSR
SOURCE: Tetrahedron (1974), 30(15), 2345-52
CODEN: TETRAB
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The conformations of the heteroanalogs I thru X of bicyclo[3.3.1]nonane were detd. from their NMR. The double chair is the preferred conformation for I thru V; O-O and O-S repulsions distorted the chair giving flattened wings. VI, IX, and X had increased proportions of boat-chair forms.
IT **54171-89-0**

RL: PRP (Properties)
(conformation of, NMR in relation to)
RN 54171-89-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)




L8 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1969:101290 CAPLUS
DOCUMENT NUMBER: 70:101290
TITLE: Metal chelates of (2-pyridyl)-substituted 3,7-diazabicyclo[3.3.1]nonanones
AUTHOR(S): Haller, Rolf
CORPORATE SOURCE: Pharm. Inst., Univ. Freiburg/Br., Freiburg/Br., Ger.
SOURCE: Arch. Pharm. (Weinheim) (1969), 302(2), 113-18
CODEN: APBDAJ
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Hot alc. L reacts with an equal molar quant. of alc. transition metal salt
to give MLX2 (M, X, R, R1, yield (%), m.p. (decompn.) given): Fe, SCN, Me,
CH2Ph, 89, -; Co, SCN, Me, CH2Ph, 74, 210-12.degree.; Cd, SCN, Me, CH2Ph, 69, 180.degree.; Ni, SCN, Et, CH2Ph, 76, 212-15.degree.; Mn, Cl, Et, Me, 71, 242.degree.. The ir spectra studied indicate that the azabicyclic complexes contain tetradentate ligands.
IT **4728-47-6**
RL: PRP (Properties)
(spectrum of, ir)
RN 4728-47-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-benzyl-9-oxo-3-phenyl-2,4-di-2-pyridyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)



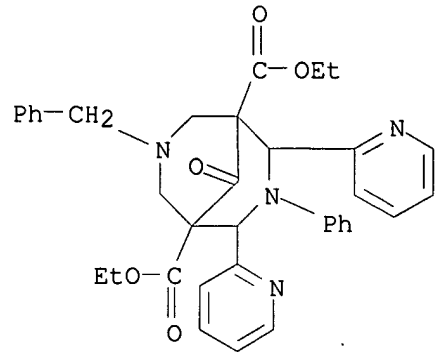
L8 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1966:35818 CAPLUS
DOCUMENT NUMBER: 64:35818
ORIGINAL REFERENCE NO.: 64:6629c-h,6630c-f
TITLE: Substituted 3,7-diaza-and 3-oxa-7-azabicyclo [3.3.1] nonanones
AUTHOR(S): Haller, R.
CORPORATE SOURCE: Univ. Freiburg/Br., Germany
SOURCE: Arzneimittel-Forsch. (1965), 15(11), 1327-30
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Substituted piperidones and tetrahydropyrones having active H groups in the 3,5-positions underwent a Mannich-type reaction with HCHO and a primary amine to form the title compds. Methyl or ethyl esters of 2,6-disubstituted-4-piperidone-3,5-dicarboxylic acid (CA 60, 15824a), (0.01 mole) were dissolved in hot EtOH, and a 20% excess of aq. HCHO, and the amine added in order, followed by an addnl. 100 ml. EtOH to effect complete soln. After standing several days, the insol. products were filtered off, or the sol. products obtained as residues, and crystd. The following I were prepd. [R2, R3, R4, % yield, m.p. (solvent) given]: Me, H, PhCH2 (Ia), 70, 184-5.degree. (MeOH); Et, H, PhCH2, 68.5, 161-2.degree. (EtOH); Me, H, Me, 68, 165.degree. (MeOH-H2O, 1:2); Et, H, Me, 35, 137.degree. (EtOH-ligroine, 1:1); Et, Me, Me, 41, 158.degree. (EtOH); Me, (CH2)2OH, PhCH2, 31, 197.degree. (MeOH); Et, (CH2)2OH, PhCH2, 22, 180.degree. (EtOH-H2O, 1:1); Et, PhCH2, PhCH2, 36, 188.degree. (EtOH); Et, Ph, PhCH2, 76, 178.degree. (EtOH); Et, H, 2-pyridylmethyl, 73, 169-70.degree. (EtOH-H2O, 1:1). II prepd. were (identification same as for I): Me, H, Me, 55.5, 154-5.degree. (EtOH-H2O, 1:1); Me, H, PhCH2, 60.5, 183.degree. (MeOH-H2O, 4:1). III, 1,5-dicarbethoxy-7-benzyl-2,4-di(3-pyridyl)-3,7-diazabicyclo[3.3.1]nonan-9-one, 75%, m. 183.degree. (EtOH), was similarly prepd. A soln. of 10.7 g. pyridine-2-carboxaldehyde, and 4 g. 2-aminoethanol in 30 ml. MeOH was treated with 8.7 g. diethyl acetonedicarboxylate, 20 ml. ether was added, and the mixt. kept 1 day to give 67% diethyl 1-(2-hydroxyethyl)-2,6-di(2-pyridyl)-4-

piperidone-3,5-dicarboxylate (IV) 67%, m. 146.degree. (decompn.) (MeOH). The corresponding diethyl ester (V) (53), m. 113-14.degree. (decompn.) (EtOH-H2O, 1:1), was similarly prepd. as was 87.5% diethyl 1-phenyl-2,6-di(2-pyridyl)-4-piperidone-3,5-dicarboxylate (VI), m. 139.degree. (decompn.) (EtOH), using aniline in place of 2-aminoethanol. IV-VI gave an intense red-violet color with alc. FeCl3. Diethyl 2,6-di(2-pyridyl)-4-piperidone-3,5-dicarboxylate (loc. cit.) (2 g.), was acetylated with 1.5 g. AcCl in 60 ml. benzene in the presence of 2 g. CaCO3 to yield 90% diethyl 1-acetyl-2,6-di(2-pyridyl)-4-piperidone-3,5-dicarboxylate (VII), m. 126.degree. (decompn.) (EtOH-H2O). VII (5 millimoles) was treated with HCHO and amines in a manner similar to the prepn. of I-III to yield 7-substituted-1,5-dicarbethoxy-2,4-di(2-pyridyl)-3-acetyl-3,7-diazabicyclo [3.3.1] nonan-9-ones (VIII) as follows [R4, % yield, m.p. (solvent) given]: H, 45, 197.degree. (decompn.) (EtOH-H2O, 2:1); Me, 53, 130.degree. (decompn.) (EtOH-H2O, 2:1); PhCH2, 70, 170.degree. (decompn.) (EtOH). Esters of 2,6-diphenyltetrahydro-4-pyrone-3,5-dicarboxylic acid (0.01 mole), were treated with HCHO and amines in the same manner as for I-III to form derivs. (IX) of 2,4-diphenyl-3-oxa-7-azabicyclo[3.3.1]nonan-9-one. IX prepd. were [R1, R2, % yield, m.p. (EtOH) given]: Et, allyl, 72, 131-2.degree.; Et, PhCH2, 57, 129.degree.; Me, 2-pyridylmethyl, 54, 181-3.degree.; Et, 2-pyridylmethyl, 49, 161.degree.. Derivs. (X) of 2,4-di(2-pyridyl)-3-thia-7-azabicyclo[3.3.1]nonan-9-one were similarly prepd., starting with the Me or Et esters of 1-thia-2,6-di(2-pyridyl)cyclohexan-4-one-3,5-dicarboxylic acid (CA 63, 5613h). X prepd. (identification same as IX) were: Me, 2-pyridylmethyl, 37, 185.degree. (decompn.) (EtOH-H2O, 2:1); Et, 2-pyridylmethyl, 35,193.degree. (decompn.) (EtOH-H2O, 2:1). A soln. of 0.7 g. Co(NO3)2.6H2O in 20 ml. EtOH was added to a hot soln. of Ia in 40 ml. EtOH and the mixt. heated 10 min. on a steam bath; the pptd. Co chelate was only slightly sol. in H2O, practically insol. in org. solvents, dimethylformamide, and dimethyl sulfoxide, decompd. 230-5.degree., yield 70%. A hot soln. of 0.6 g. KSCN and 0.6 g. MnCl2.4H2O in 30 ml. EtOH was heated on a steam bath; the pptd. KCl was filtered off, and the soln. mixed with 1 g. Ia in 40 ml. EtOH, and heated 5 min. After several hrs. standing, yellow-gold crystals of the Ia-Mn-(SCN)2 chelate pptd., 82%, decompd. 185.degree. Am. 200.degree.. IV-VI were characterized by ir spectra as enol forms; the structures of the I-III series of compds. were confirmed by N.M.R.

IT **4728-47-6**, 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-benzyl-9-oxo-3-phenyl-2,4-di-2-pyridyl-, diethyl ester
(prepn. of)

RN 4728-47-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-benzyl-9-oxo-3-phenyl-2,4-di-2-pyridyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)



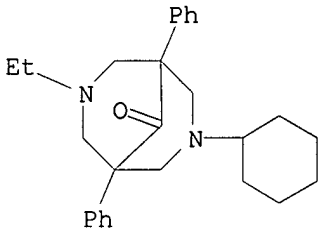
L8 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1965:480662 CAPLUS
DOCUMENT NUMBER: 63:80662
ORIGINAL REFERENCE NO.: 63:14864a-e
TITLE: Synthesis of 1,5-diphenylbispidin-9-ones. VIII. 1,5-Diphenyl-3,7-dialkylbispidin-9-ones. Asymmetrically substituted derivatives
AUTHOR(S): Chiavarelli, S.; Toeffler, H. F.; Fennoy, L. V.; Landi-Vittory, R.; Mazzeo, P.
CORPORATE SOURCE: Ist. Super. Sanita, Rome
SOURCE: Farmaco (Pavia), Ed. Sci. (1965), 20(6), 408-20
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB A series of asym. substituted 1,5-diphenyl-3,7-dialkylbispidin-9-ones (I) was prepd. from 1,3-diphenylacetone (II), paraformaldehyde (III), and acetates of primary alkylamines. An alc. soln. of 0.1 mole II, 0.4 mole III, 0.1 mole RNH2.AcOH, and 0.1 mole R'NH2.AcOH was refluxed 6-16 hrs., according to the employed amine. The reaction mixt. was cooled, dild. with an equal vol. H2O, alkalized to pH 8 with 20% Na2CO3, kept overnight, filtered, and the ppt. crystd. if solid, or purified through the perchlorate, if liquid. The reaction product consisted of a mixt. of sym. and asym. substituted I, not separable by crystn., but only by thin layer chromatography. The following I were prepd. and crystd. after chromatographic sepn. (R, R', m.p., and % yield given): Et, cyclohexyl, 132-3.degree., 43; Me, PhCH2, 132-4.degree., 48; Et, PhCH2, 129-31.degree., 44; Et, Ph(CH2)2, 131-3.degree., 50; Me, Et, 116-18.degree., 57; Et, Pr, 106-8.degree., 47; Et, iso-Pr, 140-2.degree., 41; Pr, iso-Pr, 126-8.degree., 37; Me, iso-Pr, 111-113.degree., 34. Rf and ir spectra of all the compds. are recorded. IX. 1,5-Diphenyl-3,7bis(hydroxyalkyl)- and 1,5-diphenyl-3,7-bis(methoxyalkyl)bispidin-9-ones, symmetric and asymmetric. S. Chiavarelli, H. F. Toeffler, R. Landi-Vittory, and P. Mazzeo. Ibid. 421-7. Sym. and asym. 1,5-diphenyl-3,7-bis(hydroxyalkyl)- and 1,5diphenyl-3,7-bis(methoxyalkyl)bispidin-9-ones (I) were prepd. by a general reaction from 1,3-diaryl-2-propanone, paraformaldehyde, and primary amine acetates.

A mixt. of 0.1 mole 1,3diphenyl-2-propanone, 0.4 mole paraformaldehyde, 0.1 mole RNH2.AcOH, and 0.1 mole R'NH2.AcOH in 100 ml. alc. was refluxed 6-42 hrs., according to the employed amine, cooled, dild. with equal vol. H2O, alkalized to pH 8-9 with 20% Na2CO3, kept overnight in the cold, filtered, and the ppt. crystd., if solid or purified through perchlorates and hydrochlorides, if liquid. The following sym. I were prepd. (salt, R = R', m.p., and % yield given): -, (CH2)2OCH3, 90-1.degree., 71; -, (CH2)3OCH3, 78-9.degree., 53; perchlorate 0.5-H2O, (CH2)3OH, 94-6.degree. (anhyd. m. 148-9.degree.), 47; -, (CH3)2CCH2OH, 187-8.degree., 34; hydrochloride, (CH2)3OH, 191-3.degree. (decompn.), 36; perchlorate, 3,4,5-trimethoxyphenethyl, 204-6.degree., 35. The asym. I were obtained (R, R', m.p., and % yield given): (CH2)2OCH3, CH2Ph, 101-3%, 42; (CH2)3OCH3, cyclopentanyl, 118-20.degree., 35. The ir spectra were reported. Also reported were the results of preliminary toxicological tests, which showed that the activity of I decreased rapidly with increasing of length of the substituent chain in the 3- and 7-position.

IT **4208-17-7**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclohexyl-7-ethyl-1,5-diphenyl- **4208-32-6**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclohexyl-1,5-diphenyl- **4478-45-9**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclopentyl-7-(3-methoxypropyl)-1,5-diphenyl-
(prepn. of)

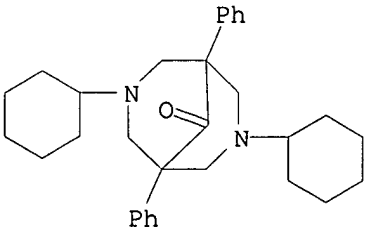
RN 4208-17-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclohexyl-7-ethyl-1,5-diphenyl- (7CI, 8CI) (CA INDEX NAME)




RN 4208-32-6 CAPLUS

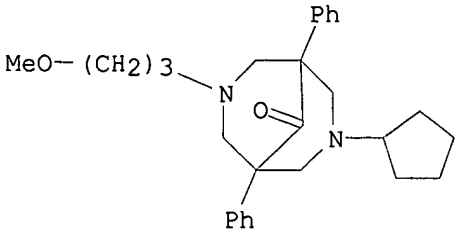
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclohexyl-1,5-diphenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)



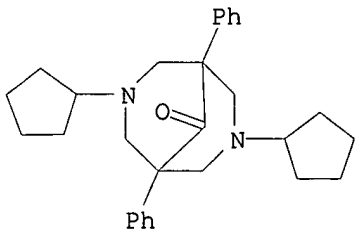

RN 4478-45-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclopentyl-7-(3-methoxypropyl)-1,5-

diphenyl- (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1965:90941 CAPLUS
DOCUMENT NUMBER: 62:90941
ORIGINAL REFERENCE NO.: 62:16251g-h,16252a
TITLE: Synthesis of 1,5-diphenylbispidin-9-ones. VII. Symmetrical 1,5-diphenyl-3,7-dialkylbispidones
AUTHOR(S): Chiavarelli, Stefano; Toeffler, Federico; Vittory, Rodolfo Landi; Mazzeo, Pietro
CORPORATE SOURCE: Ist. Super Sanita, Rome
SOURCE: Gazz. Chim. Ital. (1964), 94(10), 1021-7
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB cf. CA 56, 12900c. Correction of CA 62, 9135h. The title compds. (I) were obtained by the Mannich reaction on (PhCH2)2CO (II) and a primary or cycloalkylamine acetate in the presence of CH2O. Thus, 12.6 g. II, 7.2. g. CH2O, and 21 g. heptylamine acetate in 100 ml. MeOH refluxed 17 hrs. gave 45% I (R = C7H15) perchlorate, m. 122-4.degree. (MeOH). Similarly were obtained the following I (R, % yield, and m.p. given): C8H17, 51, --(HClO4 salt m. 116-18.degree.); iso-C8H17, 58, 89-91.degree.; C10H21, 38, --(HClO4 salt m. 126-8.degree.); C17H35, 69, 67-8.degree.; C18H37, 56,
56-8.degree.; cyclopentyl, 62, 156-8.degree..
IT **3168-98-7**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclopentyl-1,5-diphenyl-
(prepn. of)
RN 3168-98-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclopentyl-1,5-diphenyl- (7CI, 8CI) (CA INDEX NAME)



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L4               STRUCTURE UPLOADED
L5               QUE L4
L6             5 S L4
L7           100 S L6 FUL

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L8            28 S L7

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